SYMMETRIZED PERTURBATION DETERMINANTS AND APPLICATIONS TO BOUNDARY DATA MAPS AND KREIN-TYPE RESOLVENT FORMULAS

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Dedicated to the memory of Pierre Duclos (1948–2010)

Abstract. The aim of this paper is twofold: On one hand we discuss an abstract approach to symmetrized Fredholm perturbation determinants and an associated trace formula for a pair of operators of positive-type, extending a classical trace formula.

On the other hand, we continue a recent systematic study of boundary data maps in [14], that is, 2×2 matrix-valued Dirichlet-to-Neumann and more generally, Robin-to-Robin maps, associated with one-dimensional Schrödinger operators on a compact interval $[0, R]$ with separated boundary conditions at 0 and R. One of the principal new results in this paper reduces an appropriately symmetrized (Fredholm) perturbation determinant to the 2×2 determinant of the underlying boundary data map. In addition, as a concrete application of the abstract approach in the first part of this paper, we establish the trace formula for resolvent differences of self-adjoint Schrödinger operators corresponding to different (separated) boundary conditions in terms of boundary data maps.

1. Introduction

In his joint 1983 paper [15] with Jean-Michel Combes and Ruedi Seiler, Pierre Duclos considered various one-dimensional Dirichlet and Neumann Schrödinger operators and associated Krein-type resolvent formulas to study the classical limit of discrete eigenvalues in a multiple-well potential. One of the principal aims of the present paper is to consider related Krein-type resolvent formulas for general separated boundary conditions on a compact interval and establish connections with recently established boundary data maps in [14], perturbation determinants, and trace formulas. In addition, we discuss an abstract approach to symmetrized (Fredholm) perturbation determinants and an associated trace formula for a pair of operators of positive-type, extending a classical trace formula for perturbation determinants described by Gohberg and Krein [33, Sect. IV.3].

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In Section 2 we depart from our consideration of Schrödinger operators on a compact interval and turn our attention to an abstract result on symmetrized (Fredholm) determinants of the form

$$\det_{\mathcal{H}}\Big(\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\Big) \tag{1.1}$$

associated with a pair of operators (A, A_0) of positive-type (and z in appropriate sectors of the complex plane). In particular, this permits a discussion of sectorial (and hence non-self-adjoint) operators. It also naturally permits a study of self-adjoint operators (A, A_0), where A is a small form perturbation of A_0, extending the traditional case in which A is a small (Kato–Rellich-type) operator perturbation of A_0. Our principal result in Section 2 then concerns a proof of the trace formula

$$\begin{aligned} &-\frac{d}{dz}\ln\Big(\det_{\mathcal{H}}\Big(\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\Big)\Big) \\ &\quad = \operatorname{tr}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big), \end{aligned} \tag{1.2}$$

an extension of the well-known operator perturbation case in which the symmetrized expression

$$\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}} \tag{1.3}$$

is replaced by the traditional expression

$$(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1} \tag{1.4}$$

on the left-hand side of (1.2) (cf. Gohberg and Krein [33, Sect. IV.3]). The generalized trace formula (1.2) appears to be without precedent under our general hypothesis that A and A_0 are operators of positive-type and hence seems to be of independent interest.

Returning to the second principal aim of this paper, the discussion of boundary data maps for Schrödinger operators on a compact interval with separated boundary conditions, let $R > 0$, introduce the strip $S_{2\pi} = \{z \in \mathbb{C} \,|\, 0 \leq \operatorname{Re}(z) < 2\pi\}$, and consider the boundary trace map

$$\gamma_{\theta_0,\theta_R} \colon \begin{cases} C^1([0,R]) \to \mathbb{C}^2, \\ u \mapsto \begin{bmatrix} \cos(\theta_0)u(0) + \sin(\theta_0)u'(0) \\ \cos(\theta_R)u(R) - \sin(\theta_R)u'(R) \end{bmatrix}, \end{cases} \qquad \theta_0, \theta_R \in S_{2\pi}, \tag{1.5}$$

where "prime" denotes d/dx. In addition, assuming that

$$V \in L^1((0,R);dx) \tag{1.6}$$

(V is not assumed to be real-valued in Sections 1 and 3), one can introduce the family of one-dimensional Schrödinger operators H_{θ_0,θ_R} in $L^2((0,R);dx)$ by

$$\begin{aligned} &H_{\theta_0,\theta_R} f = -f'' + Vf, \quad \theta_0, \theta_R \in S_{2\pi}, \\ &f \in \operatorname{dom}(H_{\theta_0,\theta_R}) = \big\{g \in L^2((0,R);dx) \,\big|\, g, g' \in AC([0,R]);\ \gamma_{\theta_0,\theta_R}(g) = 0; \\ &\hspace{6cm} (-g'' + Vg) \in L^2((0,R);dx)\big\}, \end{aligned} \tag{1.7}$$

where $AC([0,R])$ denotes the set of absolutely continuous functions on $[0,R]$.

Assuming that $z \in \mathbb{C}\backslash\sigma(H_{\theta_0,\theta_R})$ (with $\sigma(T)$ denoting the spectrum of T) and $\theta_0, \theta_R \in S_{2\pi}$, we recall that the boundary value problem given by

$$-u'' + Vu = zu, \quad u, u' \in AC([0,R]), \tag{1.8}$$

$$\gamma_{\theta_0,\theta_R}(u) = \begin{bmatrix} c_0 \\ c_R \end{bmatrix} \in \mathbb{C}^2, \tag{1.9}$$

has a unique solution denoted by $u(z,\cdot) = u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))$ for each $c_0, c_R \in \mathbb{C}$. To each boundary value problem (1.8), (1.9), we now associate a family of *general boundary data maps*, $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) : \mathbb{C}^2 \to \mathbb{C}^2$, for $\theta_0, \theta_R, \theta_0', \theta_R' \in S_{2\pi}$, where

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) \begin{bmatrix} c_0 \\ c_R \end{bmatrix} &= \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\big(\gamma_{\theta_0,\theta_R}(u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R)))\big) \\ &= \gamma_{\theta_0',\theta_R'}(u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))). \end{aligned} \tag{1.10}$$

With $u(z,\cdot) = u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))$, $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ can be represented as a 2×2 complex matrix, where

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) \begin{bmatrix} c_0 \\ c_R \end{bmatrix} &= \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) \begin{bmatrix} \cos(\theta_0)u(z,0) + \sin(\theta_0)u'(z,0) \\ \cos(\theta_R)u(z,R) - \sin(\theta_R)u'(z,R) \end{bmatrix} \\ &= \begin{bmatrix} \cos(\theta_0')u(z,0) + \sin(\theta_0')u'(z,0) \\ \cos(\theta_R')u(z,R) - \sin(\theta_R')u'(z,R) \end{bmatrix}. \end{aligned} \tag{1.11}$$

The map $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$, $z \in \mathbb{C}\backslash\sigma(H_{\theta_0,\theta_R})$, was the principal object studied in the recent paper [14].

In Section 3 we recall the principal results of [14] most relevant to the present investigation. More precisely, we review the basic properties of $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$, and detail the explicit representation of the boundary data maps $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ in terms of the resolvent of the underlying Schrödinger operator H_{θ_0,θ_R}. We discuss the associated boundary trace maps, associated linear fractional transformations relating the boundary data maps $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ and $\Lambda_{\delta_0,\delta_R}^{\delta_0',\delta_R'}(z)$ and mention the fact that $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot)$ is a matrix-valued Herglotz function (i.e., analytic on $\mathbb{C}_+$, the open complex upper half-plane, with a nonnegative imaginary part) in the special case where H_{θ_0,θ_R} is self-adjoint. We conclude our review of [14] with Krein-type resolvent formulas explicitely relating the resolvents of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$.

In Section 4, we focus on the second group of new results in this paper and relate $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ with the trace formula for the difference of resolvents of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ and the underlying perturbation determinants. In this context we will be assuming self-adjointness of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$. More precisely, we will prove the following facts:

$$\begin{aligned} &{\det}_{L^2((0,R);dx)}\Big(\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}}\Big) \\ &\quad = \frac{\sin(\theta_0)\sin(\theta_R)}{\sin(\theta_0')\sin(\theta_R')} {\det}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big), \\ &\quad \theta_0,\theta_R \in [0,2\pi),\ \theta_0',\theta_R' \in (0,2\pi)\backslash\{\pi\},\ z \in \rho(H_{\theta_0,\theta_R}), \end{aligned} \tag{1.12}$$

and

$$\begin{aligned} &{\operatorname{tr}}_{L^2((0,R);dx)}\big((H_{\theta_0',\theta_R'} - zI)^{-1} - (H_{\theta_0,\theta_R} - zI)^{-1}\big) \\ &\quad = -\frac{d}{dz}\ln\Big({\det}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)\Big), \quad z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{\theta_0',\theta_R'}). \end{aligned} \tag{1.13}$$

For classical as well as recent fundamental literature on Weyl–Titchmarsh operators (i.e., spectral parameter dependent Dirichlet-to-Neumann maps, or more

generally, Robin-to-Robin maps, resp., Poincaré–Steklov operators), relevant in the context of boundary value spaces (boundary triples, etc.), we refer, for instance, to [3]– [18], [26]–[29], [34], [35, Ch. 13], [62]–[64], [65], [66], and especially, to the extensive bibliography in [14].

Finally, we briefly summarize some of the notation used in this paper: Let $\mathcal{H}$ be a separable complex Hilbert space, $(\cdot,\cdot)_{\mathcal{H}}$ the scalar product in $\mathcal{H}$ (linear in the second argument), and $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$. Next, let T be a linear operator mapping (a subspace of) a Banach space into another, with $\operatorname{dom}(T)$ and $\ker(T)$ denoting the domain and kernel (i.e., null space) of T. The closure of a closable operator S is denoted by $\overline{S}$. The spectrum essential spectrum, discrete spectrum, and resolvent set of a closed linear operator in $\mathcal{H}$ will be denoted by $\sigma(\cdot)$. $\sigma_{\rm ess}(\cdot)$, $\sigma_{\rm d}(\cdot)$, and $\rho(\cdot)$, respectively. The Banach space of bounded linear operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$, the analogous notation $\mathcal{B}(\mathcal{X}_1,\mathcal{X}_2)$, will be used for bounded operators between two Banach spaces $\mathcal{X}_1$ and $\mathcal{X}_2$. The Banach space of compact operators defined on $\mathcal{H}$ is denoted by $\mathcal{B}_\infty(\mathcal{H})$ and the ℓ^p-based trace ideals are denoted by $\mathcal{B}_p(\mathcal{H})$, $p\geq 1$. The Fredholm determinant for trace class perturbations of the identity in $\mathcal{H}$ is denoted by $\det_{\mathcal{H}}(\cdot)$, the trace for trace class operators in $\mathcal{H}$ will be denoted by $\operatorname{tr}_{\mathcal{H}}(\cdot)$.

2. Symmetrized Perturbation Determinants and Trace Formulas: An Abstract Approach

In this section we present our first group of new results, the connection between appropriate perturbation determinants and trace formulas in an abstract setting. Throughout this section, $\mathcal{H}$ denotes a complex, separable Hilbert space with inner product $(\cdot,\cdot)_{\mathcal{H}}$, and $I_{\mathcal{H}}$ represents the identity operator in $\mathcal{H}$. For basic facts on trace ideals and infinite determinants we refer, for instance, to [31]–[33], [68], and [69].

We start with the following classical result:

Theorem 2.1 ([33], p. 163)**.** *Let $T(\cdot)$ be analytic in the $\mathcal{B}_1(\mathcal{H})$-norm on some open set $\Omega\subseteq\mathbb{C}$. Then $\det_{\mathcal{H}}(I_{\mathcal{H}}+T(\cdot))$ is analytic in Ω and*

$$\begin{aligned} \frac{d}{dz}\ln(\det{}_{\mathcal{H}}(I_{\mathcal{H}}+T(z))) &= \operatorname{tr}_{\mathcal{H}}\big((I_{\mathcal{H}}+T(z))^{-1}T'(z)\big), \\ & z\in\big\{\zeta\in\Omega \,\big|\, (I_{\mathcal{H}}+T(\zeta))^{-1}\in\mathcal{B}(\mathcal{H})\big\}. \end{aligned} \tag{2.1}$$

Next, we recall a classical special case in connection with standard perturbation determinants (cf. [33, Ch. IV]):

Theorem 2.2 ([33], Sect. IV.3, [47])**.** *Assume that A and A_0 are densely defined, closed, linear operators in $\mathcal{H}$ satisfying*

$$\operatorname{dom}(A_0)\subseteq\operatorname{dom}(A), \tag{2.2}$$

$$\begin{aligned} &(A-zI_{\mathcal{H}})\big[(A-zI_{\mathcal{H}})^{-1}-(A_0-zI_{\mathcal{H}})^{-1}\big]\in\mathcal{B}_1(\mathcal{H}) \ \textit{for some} \\ &\qquad\qquad (\textit{and hence for all}) \ z\in\rho(A)\cap\rho(A_0)\big). \end{aligned} \tag{2.3}$$

Then

$$\begin{aligned} -\frac{d}{dz}\ln\big(\det{}_{\mathcal{H}}\big((A-zI_{\mathcal{H}})(A_0-zI_{\mathcal{H}})^{-1}\big)\big) &= \operatorname{tr}_{\mathcal{H}}\big((A-zI_{\mathcal{H}})^{-1}-(A_0-zI_{\mathcal{H}})^{-1}\big), \\ & z\in\rho(A)\cap\rho(A_0). \end{aligned} \tag{2.4}$$

Proof. For completeness, and since we intend to extend this type of result to certain quadratic form perturbations, we briefly sketch the proof of (2.4). Pick $z \in \rho(A) \cap \rho(A_0)$. Since assumption (2.3) is equivalent to

$$-(A - zI_{\mathcal{H}})\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big] = (A - A_0)(A_0 - zI_{\mathcal{H}})^{-1} \in \mathcal{B}_1(\mathcal{H}), \quad (2.5)$$

the identity

$$(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1} = I_{\mathcal{H}} + (A - A_0)(A_0 - zI_{\mathcal{H}})^{-1} \quad (2.6)$$

shows that $\det_{\mathcal{H}}\big((A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big)$ is well-defined and analytic for $z \in \rho(A_0)$. Incidentally, (2.5) also yields that if (2.3) is satisfied for some $z \in \rho(A) \cap \rho(A_0)$, then it is satisfied for all $z \in \rho(A) \cap \rho(A_0)$. An application of (2.1) and cyclicity of the trace (i.e., $\operatorname{tr}_{\mathcal{H}}(ST) = \operatorname{tr}_{\mathcal{H}}(TS)$ whenever $S, T \in \mathcal{B}(\mathcal{H})$ with $ST, TS \in \mathcal{B}_1(\mathcal{H})$) imply

$$\begin{aligned}
&-\frac{d}{dz}\ln\big(\det_{\mathcal{H}}\big((A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big)\big) \\
&\quad = -tr_{\mathcal{H}}\Big(\big\{(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big\}^{-1}\big[(A - A_0)(A_0 - zI_{\mathcal{H}})^{-1}\big]'\Big) \\
&\quad = -tr_{\mathcal{H}}\Big(\big\{(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big\}^{-1}(A - A_0)(A_0 - zI_{\mathcal{H}})^{-2}\Big) \\
&\quad = -tr_{\mathcal{H}}\Big((A_0 - zI_{\mathcal{H}})^{-1}\big\{(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big\}^{-1}(A - A_0)(A_0 - zI_{\mathcal{H}})^{-1}\Big) \\
&\quad = tr_{\mathcal{H}}\Big((A_0 - zI_{\mathcal{H}})^{-1}\big\{(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big\}^{-1} \\
&\qquad\qquad \times (A - zI_{\mathcal{H}})\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big]\Big) \\
&\quad = tr_{\mathcal{H}}\Big((A_0 - zI_{\mathcal{H}})^{-1}\big\{(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big\}^{-1}\big\{(A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big\} \\
&\qquad\qquad \times (A_0 - zI_{\mathcal{H}})\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big]\Big) \\
&\quad = tr_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big). \qquad (2.7)
\end{aligned}$$

□

For an extension of Theorem 2.2, applicable, in particular, to suitable quadratic form perturbations, we briefly recall a few basic facts on operators of positive-type and their fractional powers. While this theory has been fully developed in connection with complex Banach spaces, we continue to restrict ourselves here to the case of complex, separable Hilbert spaces. For details on this theory we refer, for instance, to [36, Chs. 2, 3, 7], [42, Ch. 4], [53, Ch. 4], [56, Chs. 1, 3–5], and [74, Chs. 2, 16].

Definition 2.3. Let A be a densely defined, closed, linear operator in $\mathcal{H}$ and denote by $S_\omega \subset \mathbb{C}$, $\omega \in [0, \pi)$, the open sector

$$S_\omega = \begin{cases} \{z \in \mathbb{C} \,|\, z \neq 0, \, |\arg(z)| < \omega\}, & \omega \in (0, \pi), \\ (0, \infty), & \omega = 0, \end{cases} \quad (2.8)$$

with vertex at $z = 0$ along the positive real axis and opening angle 2ω.
(i) A is said to be of *nonnegative-type* if

$$\begin{aligned} &(\alpha) \;\; (-\infty, 0) \subset \rho(A), \\ &(\beta) \;\; M(A) = \sup_{t>0} \big\| t(A + tI_{\mathcal{H}})^{-1} \big\|_{\mathcal{B}(\mathcal{H})} < \infty. \end{aligned} \quad (2.9)$$

(ii) A is said to be of *positive-type* if

$$\begin{aligned} &(\alpha)\ \ (-\infty,0]\subset\rho(A),\\ &(\beta)\ \ M_A=\sup_{t\geq 0}\big\|(1+t)(A+tI_{\mathcal H})^{-1}\big\|_{\mathcal B(\mathcal H)}<\infty. \end{aligned} \tag{2.10}$$

(iii) A is called sectorial of angle $\omega\in[0,\pi)$, denoted by $A\in\operatorname{Sect}(\omega)$, if

$$\begin{aligned} &(\alpha)\ \ \sigma(A)\subseteq\overline{S_\omega},\\ &(\beta)\ \text{For all } \omega'\in(\omega,\pi),\ M(A,\omega')=\sup_{z\in\mathbb C\backslash\overline{S_{\omega'}}}\big\|z(A-zI_{\mathcal H})^{-1}\big\|_{\mathcal B(\mathcal H)}<\infty. \end{aligned} \tag{2.11}$$

(iv) A is called *quasi-sectorial of angle* $\omega\in[0,\pi)$ *if there exists* $t_0\in\mathbb R$ *such that* $A+t_0I_{\mathcal H}$ *is sectorial of angle* $\omega\in[0,\pi)$. *In this context we introduce the shifted sector* $-t_0+S_\omega$*, where*

$$-t_0+S_\omega=\begin{cases}\{z\in\mathbb C\,|\,z\neq -t_0,\ |\arg(-t_0+z)|<\omega\}, & \omega\in(0,\pi),\\ (-t_0,\infty), & \omega=0.\end{cases} \tag{2.12}$$

Next, we recall a number of useful facts:

(I) If A is of nonnegative-type, then (cf., e.g., [36, Proposition 2.1.1 a)])

$$M(A)\geq 1\ \text{ and }\ A\in\operatorname{Sect}(\pi-\arcsin(1/M(A))). \tag{2.13}$$

Moreover, if A is of nonnegative-type (resp., of positive-type) then

$$A+tI_{\mathcal H}\ \text{ is of nonnegative-type (resp., of positive-type) for all } t>0. \tag{2.14}$$

If A is of positive-type, then (cf., e.g., [53, Lemma 4.2])

$$\{z\in\mathbb C\,|\,\mathrm{Re}(z)\leq 0,\ |\mathrm{Im}(z)|<(|\mathrm{Re}(z)|+1)/M_A\}\cup\{z\in\mathbb C\,|\,|z|<1/M_A\}\subset\rho(A), \tag{2.15}$$

and for every $\omega_0\in(0,\arctan(1/M_A))$, $r_0\in(0,1/M_A)$, there exists $M_0(A,\omega_0,r_0)>0$ such that

$$\begin{aligned} &\|(A-zI_{\mathcal H})^{-1}\|_{\mathcal B(\mathcal H)}\leq\frac{M_0(A,\omega_0,r_0)}{1+|z|},\\ &z\in\{\zeta\in\mathbb C\,|\,\mathrm{Re}(\zeta)<0,\ |\mathrm{Im}(\zeta)|/|\mathrm{Re}(\zeta)|\leq\tan(\omega_0)\}\cup\{\zeta\in\mathbb C\,|\,|\zeta|\leq r_0\}. \end{aligned} \tag{2.16}$$

(II) If $A\in\operatorname{Sect}(\omega)$ for some $\omega\in[0,\pi)$ and $\ker(A)=\{0\}$, then (cf., e.g., [36, Proposition 2.1.1 b)])

$$A^{-1}\in\operatorname{Sect}(\omega)\ \text{ and }\ M\big(A^{-1},\omega'\big)\leq M(A,\omega')+1,\quad \omega'\in(\omega,\pi). \tag{2.17}$$

(III) If $A\in\operatorname{Sect}(\omega)$ for some $\omega\in[0,\pi)$, then (cf., e.g., [36, Proposition 2.1.1 j)])

$$A^*\in\operatorname{Sect}(\omega)\ \text{ and }\ M(A^*,\omega')=M(A,\omega'),\quad \omega'\in(\omega,\pi). \tag{2.18}$$

(IV) Suppose A is of positive-type then (cf., e.g., [42, p. 280])

$$A^{-\alpha}=\frac{\sin(\pi\alpha)}{\pi}\int_0^\infty dt\,t^{-\alpha}(A+tI_{\mathcal H})^{-1}\in\mathcal B(\mathcal H),\quad 0<\mathrm{Re}(\alpha)<1. \tag{2.19}$$

(In this context of bounded operators $A^{-\alpha}$, $0<\alpha<1$, and integrands bounded in norm by a Lebesgue integrable function, the integral in (2.19) and in analogous

situations in this section, is viewed as a norm convergent Bochner integral.) Moreover, $A^{-\alpha}$ has an analytic continuation to the strip $0 < \operatorname{Re}(\alpha) < n+1$, $n \in \mathbb{N}$, given by

$$A^{-\alpha} = \frac{\sin(\pi\alpha)}{\pi} \frac{n!}{(1-\alpha)(2-\alpha)\cdots(n-\alpha)} \int_0^\infty dt\, t^{n-\alpha}(A + tI_{\mathcal{H}})^{-n-1} \in \mathcal{B}(\mathcal{H}), \quad 0 < \operatorname{Re}(\alpha) < n+1. \tag{2.20}$$

In particular,

$$A^{-\alpha} = \frac{\sin(\pi\alpha)}{\pi(1-\alpha)} \int_0^\infty dt\, t^{1-\alpha}(A + tI_{\mathcal{H}})^{-2} \in \mathcal{B}(\mathcal{H}), \quad 0 < \operatorname{Re}(\alpha) < 2. \tag{2.21}$$

We also note that if $A \in \operatorname{Sect}(\omega)$ and $\alpha \in (0,1)$, then (cf., e.g., [36, Remark 3.1.16]) $A^\alpha \in \operatorname{Sect}(\alpha\omega)$, $M(A^\alpha) \leq M(A)$, and

$$(A^\alpha - zI_{\mathcal{H}})^{-1} = \frac{\sin(\pi\alpha)}{\pi} \int_0^\infty dt\, \frac{t^\alpha}{(z - t^\alpha e^{i\pi\alpha})(z - t^\alpha e^{-i\pi\alpha})} (A + tI_{\mathcal{H}})^{-1}, \quad |\arg(z)| > \alpha\pi. \tag{2.22}$$

(V) Suppose A is of positive-type and $0 < \operatorname{Re}(\alpha) < n$ for some $n \in \mathbb{N}$, then (cf., e.g., [53, Definition 4.5])

$$A^\alpha f = A^n A^{\alpha - n} f, \quad f \in \operatorname{dom}(A^\alpha) = \{g \in \mathcal{H} \,|\, A^{\alpha-n} g \in \operatorname{dom}(A^n)\}. \tag{2.23}$$

Moreover,

$$\operatorname{dom}(A^\alpha) = \operatorname{ran}(A^{-\alpha}) \text{ and } A^\alpha = (A^{-\alpha})^{-1}, \quad \operatorname{Re}(\alpha) > 0. \tag{2.24}$$

In particular, since $A^{-\alpha} \in \mathcal{B}(\mathcal{H})$,

$$A^\alpha \text{ is closed in } \mathcal{H} \text{ for all } \operatorname{Re}(\alpha) > 0. \tag{2.25}$$

(VI) Suppose A is of positive-type and $\operatorname{Re}(\alpha_1) > 0$, $\operatorname{Re}(\alpha_2) > 0$, then (cf., e.g., [53, Proposition 4.4 (iv)])

$$A^{-\alpha_1} A^{-\alpha_2} = A^{-\alpha_1 - \alpha_2}. \tag{2.26}$$

(VII) Suppose A and B are of positive-type and resolvent commuting, that is,

$$\begin{gathered}(A + sI_{\mathcal{H}})^{-1}(B + tI_{\mathcal{H}})^{-1} = (B + tI_{\mathcal{H}})^{-1}(A + sI_{\mathcal{H}})^{-1} \\ \text{for some (and hence for all) } s > 0,\, t > 0.\end{gathered} \tag{2.27}$$

Then (cf., e.g., [53, p. 95])

$$\begin{aligned}&(AB)^\alpha f = A^\alpha B^\alpha f = B^\alpha A^\alpha f = (BA)^\alpha f, \\ &\quad f \in \operatorname{dom}((AB)^\alpha) = \{g \in \operatorname{dom}(B^\alpha) \,|\, B^\alpha g \in \operatorname{dom}(A^\alpha)\} \\ &\qquad = \{g \in \operatorname{dom}(A^\alpha) \,|\, A^\alpha g \in \operatorname{dom}(B^\alpha)\} = \operatorname{dom}((BA)^\alpha), \quad \alpha \in \mathbb{C}, \operatorname{Re}(\alpha) \neq 0.\end{aligned} \tag{2.28}$$

(VIII) In the special case where A is self-adjoint and strictly positive in $\mathcal{H}$ (i.e., $A \geq \varepsilon I_{\mathcal{H}}$ for some $\varepsilon > 0$), A^α, $\alpha \in \mathbb{C}\backslash\{0\}$, defined on one hand as in the case of operators of positive-type above, and on the other by the spectral theorem, coincide (cf., e.g., [53, Sect. 4.3.1], [70, Sect. 1.18.10]). In particular,

$$\operatorname{dom}(A^\alpha) = \bigg\{f \in \mathcal{H} \,\Big|\, \|A^\alpha f\|_{\mathcal{H}}^2 = \int_{[\varepsilon,\infty]} \lambda^{2\operatorname{Re}(\alpha)} d\|E_A(\lambda) f\|_{\mathcal{H}}^2 < \infty\bigg\}, \quad \alpha \in \mathbb{C}\backslash\{0\}, \tag{2.29}$$

in this case. Here $\{E_A(\lambda)\}_{\lambda\in\mathbb{R}}$ denotes the family of spectral projections of A.
(It is possible to extend some of these formulas to $\operatorname{Re}(\alpha) = 0$, but we omit the

details since this will play no role in this manuscript.)

For the remainder of this section the basic assumptions on A and A_0, extending (2.2) and (2.3), then read as follows:

Hypothesis 2.4. *Let A and A_0 be densely defined, closed, linear operators in $\mathcal{H}$.*
(i) *Suppose there exists $t_0 \in \mathbb{R}$ such that $A+t_0I_{\mathcal{H}}$ and $A_0+t_0I_{\mathcal{H}}$ are of positive-type and $(A+t_0I_{\mathcal{H}}) \in \mathrm{Sect}(\omega_0)$, $(A_0+t_0I_{\mathcal{H}}) \in \mathrm{Sect}(\omega_0)$ for some $\omega_0 \in [0,\pi)$.*
(ii) *In addition, assume that for some $t_1 \geq t_0$,*

$$\mathrm{dom}\big((A_0+t_1I_{\mathcal{H}})^{1/2}\big) \subseteq \mathrm{dom}\big((A+t_1I_{\mathcal{H}})^{1/2}\big), \tag{2.30}$$

$$\mathrm{dom}\big((A_0^*+t_1I_{\mathcal{H}})^{1/2}\big) \subseteq \mathrm{dom}\big((A^*+t_1I_{\mathcal{H}})^{1/2}\big), \tag{2.31}$$

$$\overline{(A+t_1I_{\mathcal{H}})^{1/2}\big[(A+t_1I_{\mathcal{H}})^{-1}-(A_0+t_1I_{\mathcal{H}})^{-1}\big](A+t_1I_{\mathcal{H}})^{1/2}} \in \mathcal{B}_1(\mathcal{H}). \tag{2.32}$$

One observes by item (I), there always exists $\omega_0 \in [0,\pi)$ as in Hypothesis 2.4 (i) as long as $A+t_0I_{\mathcal{H}}$ and $A_0+t_0I_{\mathcal{H}}$ are of nonnegative-type.

Our next results will show that if (2.30)–(2.32) hold for some $t_1 \geq t_0$, then they actually extend to $-t_1 = z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$:

Lemma 2.5. *Assume that A satisfy Hypothesis 2.4 (i). Then $(A+tI_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H})$ (resp., $(A^*+tI_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H})$), $t>t_0$, analytically extends to $(A-zI_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H})$ (resp., $(A^*-zI_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H})$) for $z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$. In addition,*

$$\mathrm{dom}\big((A-zI_{\mathcal{H}})^{1/2}\big) = \mathrm{dom}\big((A+t_0I_{\mathcal{H}})^{1/2}\big), \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big), \tag{2.33}$$

$$\mathrm{dom}\big((A^*-zI_{\mathcal{H}})^{1/2}\big) = \mathrm{dom}\big((A^*+t_0I_{\mathcal{H}})^{1/2}\big), \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big). \tag{2.34}$$

Proof. Applying (2.19) with $\alpha = 1/2$ and A replaced by $(A+sI_{\mathcal{H}})$, $s>t_0$, one obtains

$$(A+sI_{\mathcal{H}})^{-1/2} = \frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A+(s+t)I_{\mathcal{H}})^{-1}, \quad s>t_0. \tag{2.35}$$

The resolvent estimates in (2.10) and (2.11) then prove that $(A+sI_{\mathcal{H}})^{-1/2}$, $s>t_0$, analytically extends to $(A-zI_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H})$, $z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$, with the result

$$(A-zI_{\mathcal{H}})^{-1/2} = \frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A+(-z+t)I_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big). \tag{2.36}$$

In the following we choose z, $z_1 \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$ such that $|z_1-z| < \big\|(A-z_1I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}(\mathcal{H})}^{-1}$ and consider the resolvent identity

$$(A-zI_{\mathcal{H}}) = (A-z_1I_{\mathcal{H}})\big[I_{\mathcal{H}}+(z_1-z)(A-z_1I_{\mathcal{H}})^{-1}\big]. \tag{2.37}$$

It follows from $(A+t_0I_{\mathcal{H}}) \in \mathrm{Sect}(\omega_0)$ and (2.10), (2.11) that

$$A-zI_{\mathcal{H}},\ z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big), \text{ is of positive-type.} \tag{2.38}$$

To prove the claim (2.38) we first note that $z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$ implies that $(-\infty,0] \subset \rho(A-zI_{\mathcal{H}})$. Next, one chooses $\omega_0' \in (\omega,\pi)$ such that actually, $z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0'}}\big)$. Then

$$\begin{split} &\sup_{t\geq 0}\big\|(1+t)(A+(t-z)I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}(\mathcal{H})} \\ &\quad = \sup_{\zeta=z+t_0-t,\, t\geq 0}|(1+t)/\zeta|\big\|\zeta(A+(t_0-z)I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}(\mathcal{H})} \leq C(z)<\infty \end{split} \tag{2.39}$$

since $\sup_{t\geq 0}|(1+t)/(z+t_0-t)|<\infty$, the estimate (2.10) ($\beta$) becomes a special case of (2.11) (β).

In addition, $\big\|(z_1-z)(A-z_1I_{\mathcal H})^{-1}\big\|_{\mathcal{B}(\mathcal H)}<1$ implies that $B=I_{\mathcal H}+(z_1-z)(A-z_1I_{\mathcal H})^{-1}$ is of positive-type as well since

$$\begin{aligned}
&\big\|(1+t)(B+tI_{\mathcal H})^{-1}\big\|_{\mathcal{B}(\mathcal H)}=\Big\|(1+t)\left[(1+t)I_{\mathcal H}+(z_1-z)(A-z_1I_{\mathcal H})^{-1}\right]^{-1}\Big\|_{\mathcal{B}(\mathcal H)}\\
&\quad=\left\|\left[I_{\mathcal H}+\frac{z_1-z}{1+t}(A-z_1I_{\mathcal H})^{-1}\right]^{-1}\right\|_{\mathcal{B}(\mathcal H)}\\
&\quad\leq\Big[1-\big\|(z_1-z)(A-z_1I_{\mathcal H})^{-1}\big\|_{\mathcal{B}(\mathcal H)}\Big]^{-1}<\infty,\quad t\geq 0.
\end{aligned}\tag{2.40}$$

Thus (VII) applied to the resolvent identity (2.37) yields

$$\begin{aligned}
&(A-zI_{\mathcal H})^{-1/2}=(A-z_1I_{\mathcal H})^{-1/2}\left[I_{\mathcal H}+(z_1-z)(A-z_1I_{\mathcal H})^{-1}\right]^{-1/2},\\
&\qquad z,z_1\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big),\ |z-z_1|<\big\|(A-z_1I_{\mathcal H})^{-1}\big\|_{\mathcal{B}(\mathcal H)}^{-1}.
\end{aligned}\tag{2.41}$$

Bounded invertibility of $\left[I_{\mathcal H}+(-z+z_1)(A-z_1I_{\mathcal H})^{-1}\right]^{-1/2}$ for $z,z_1\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$, $|z-z_1|<\big\|(A-z_1I_{\mathcal H})^{-1}\big\|_{\mathcal{B}(\mathcal H)}^{-1}$ then implies that $\operatorname{ran}\big((A-zI_{\mathcal H})^{-1/2}\big)$ is locally constant in $z\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$,

$$\begin{aligned}
&\operatorname{ran}\big((A-zI_{\mathcal H})^{-1/2}\big)=\operatorname{ran}\big((A-z_1I_{\mathcal H})^{-1/2}\big),\\
&z,z_1\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big),\ |z-z_1|<\big\|(A-z_1I_{\mathcal H})^{-1}\big\|_{\mathcal{B}(\mathcal H)}^{-1},
\end{aligned}\tag{2.42}$$

and hence that

$$\operatorname{ran}\big((A-zI_{\mathcal H})^{-1/2}\big)=\operatorname{ran}\big((A-z_1I_{\mathcal H})^{-1/2}\big),\quad z,z_1\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big).\tag{2.43}$$

An application of (2.24) then gives (2.33). Equation (2.34) is proved analogously with the help of (III). □

Lemma 2.6. *Assume that A and A_0 satisfy Hypothesis 2.4 (i) and suppose that* (2.30) *and* (2.31) *hold for some $t_1\geq t_0$. Then* (2.30) *and* (2.31) *extend to*

$$\operatorname{dom}\big((A_0-zI_{\mathcal H})^{1/2}\big)\subseteq\operatorname{dom}\big((A-zI_{\mathcal H})^{1/2}\big),\quad z\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big),\tag{2.44}$$

$$\operatorname{dom}\big((A_0^*-zI_{\mathcal H})^{1/2}\big)\subseteq\operatorname{dom}\big((A^*-zI_{\mathcal H})^{1/2}\big),\quad z\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big).\tag{2.45}$$

Moreover,

$$\begin{aligned}
&(A-zI_{\mathcal H})^{1/2}(A_0-zI_{\mathcal H})^{-1/2}\in\mathcal{B}(\mathcal H)\ \text{ and }\ (A^*-zI_{\mathcal H})^{1/2}(A_0^*-zI_{\mathcal H})^{-1/2}\in\mathcal{B}(\mathcal H),\\
&\quad\text{are analytic for } z\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big) \text{ with respect to the } \mathcal{B}(\mathcal H)\text{-norm.}
\end{aligned}\tag{2.46}$$

Proof. By items (I) and (III) it again suffices to just focus on the proof of (2.44).

Since by (2.33) and (2.34) the domains of $(A-zI_{\mathcal H})^{1/2}$ and $(A^*-zI_{\mathcal H})^{1/2}$ are z-independent for $z\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$, (2.30) and (2.31) extend to $z\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big)$.

To prove the analyticity statement involving A and A_0 in (2.46) we write

$$\begin{aligned}
&(A-zI_{\mathcal H})^{1/2}(A_0-zI_{\mathcal H})^{-1/2}=\left[(A-zI_{\mathcal H})^{1/2}(A-z_0I_{\mathcal H})^{-1/2}\right]\\
&\quad\times\left[(A-z_0I_{\mathcal H})^{1/2}(A_0-z_0I_{\mathcal H})^{-1/2}\right]\left[(A_0-z_0I_{\mathcal H})^{1/2}(A_0-zI_{\mathcal H})^{-1/2}\right],\\
&\qquad\qquad z,z_0\in\mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big),
\end{aligned}\tag{2.47}$$

and separately investigate each of the three factors in (2.47). Since by hypothesis (2.33) holds for A and A_0, (2.44) yields that

$$(A - z_0 I_{\mathcal{H}})^{1/2}(A_0 - z_0 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H}). \tag{2.48}$$

Next, applying (2.41) with A replaced by A_0 yields

$$\begin{aligned}
&(A_0 - z_0 I_{\mathcal{H}})^{1/2}(A_0 - z I_{\mathcal{H}})^{-1/2} \\
&\quad = \big[(A_0 - z_0 I_{\mathcal{H}})^{1/2}(A_0 - z_1 I_{\mathcal{H}})^{-1/2}\big]\big[I_{\mathcal{H}} + (z_1 - z)(A_0 - z_1 I_{\mathcal{H}})^{-1}\big]^{-1/2}, \\
&\qquad z, z_0, z_1 \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big),\ |z - z_1| < \big\|(A - z_1 I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}(\mathcal{H})}^{-1}.
\end{aligned} \tag{2.49}$$

Since by (2.40) (with A replaced by A_0) $B = I_{\mathcal{H}} + (z_1 - z)(A_0 - z_1 I_{\mathcal{H}})^{-1}$ is of positive-type, it follows from (2.19) (with $\alpha = 1/2$ and A replaced by B) and a geometric series expansion that

$$\begin{aligned}
B^{-1/2} &= \big[I_{\mathcal{H}} + (z_1 - z)(A_0 - z_1 I_{\mathcal{H}})^{-1}\big]^{-1/2} \\
&= \frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}\big[(1+t)I_{\mathcal{H}} + (z_1 - z)(A_0 - z_1 I_{\mathcal{H}})^{-1}\big]^{-1} \\
&= \sum_{m=0}^\infty (-1)^m (z_1 - z)^m (A_0 - z_1 I_{\mathcal{H}})^{-m}\, \frac{1}{\pi}\int_0^\infty \frac{dt\, t^{-1/2}}{(1+t)^{m+1}} \\
&= \sum_{m=0}^\infty \frac{\Gamma(m + (1/2))}{\Gamma(m+1)\Gamma(1/2)} (-1)^m (z_1 - z)^m (A_0 - z_1 I_{\mathcal{H}})^{-m}.
\end{aligned} \tag{2.50}$$

Thus $\big[I_{\mathcal{H}} + (z_1 - z)(A_0 - z_1 I_{\mathcal{H}})^{-1}\big]^{-1/2}$ is analytic with respect to z for $z, z_1 \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$, $|z - z_1| < \big\|(A_0 - z_1 I_{\mathcal{H}})^{-1}\big\|_{\mathcal{B}(\mathcal{H})}^{-1}$. Moreover, by (2.33) (with A replaced by A_0), $(A_0 - z_0 I_{\mathcal{H}})^{1/2}(A_0 - z_1 I_{\mathcal{H}})^{-1/2} \in \mathcal{B}(\mathcal{H})$, and hence one concludes that the left-hand side of (2.49) is analytic with respect to $z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$.

Finally, writing

$$\begin{aligned}
&(A - z I_{\mathcal{H}})^{1/2}(A - z_0 I_{\mathcal{H}})^{-1/2} = (A - z I_{\mathcal{H}})(A - z I_{\mathcal{H}})^{-1/2}(A - z_0 I_{\mathcal{H}})^{-1/2} \\
&\quad = A(A - z I_{\mathcal{H}})^{-1/2}(A - z_0 I_{\mathcal{H}})^{-1/2} - z(A - z I_{\mathcal{H}})^{-1/2}(A - z_0 I_{\mathcal{H}})^{-1/2}
\end{aligned} \tag{2.51}$$

it suffices to focus on the term $A(A - z I_{\mathcal{H}})^{-1/2}(A - z_0 I_{\mathcal{H}})^{-1/2}$. Writing

$$\begin{aligned}
&A(A - z I_{\mathcal{H}})^{-1/2}(A - z_0 I_{\mathcal{H}})^{-1/2} \\
&\quad = \big[A(A - z_0 I_{\mathcal{H}})^{-1}\big]\big[(A - z_0 I_{\mathcal{H}})^{1/2}(A - z I_{\mathcal{H}})^{-1/2}\big],
\end{aligned} \tag{2.52}$$

employing the obvious fact that $A(A - z_0 I_{\mathcal{H}})^{-1} \in \mathcal{B}(\mathcal{H})$, the analyticity of $(A - z_0 I_{\mathcal{H}})^{1/2}(A - z I_{\mathcal{H}})^{-1/2}$ (and hence that of the left-hand sides in (2.51) and (2.52)) with respect to $z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$ then follows as in (2.49) above with A_0 replaced by A. $\square$

Lemma 2.7. *Assume that A and A_0 satisfy Hypothesis* 2.4. *Then* (2.32) *extends to*

$$\begin{aligned}
&\overline{(A - z I_{\mathcal{H}})^{1/2}\big[(A - z I_{\mathcal{H}})^{-1} - (A_0 - z I_{\mathcal{H}})^{-1}\big](A - z I_{\mathcal{H}})^{1/2}} \in \mathcal{B}_1(\mathcal{H}), \\
&\hspace{6cm} z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big).
\end{aligned} \tag{2.53}$$

In addition, $\overline{(A - z I_{\mathcal{H}})^{1/2}\big[(A - z I_{\mathcal{H}})^{-1} - (A_0 - z I_{\mathcal{H}})^{-1}\big](A - z I_{\mathcal{H}})^{1/2}}$ *is analytic for* $z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$ *with respect to the* $\mathcal{B}_1(\mathcal{H})$*-norm.*

Proof. Let $z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$ and $t_1 \geq t_0$ as in (2.32). Using the fact

$$\begin{aligned}(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1} &= (A + t_1 I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1}\\ &\quad \times \big[(A + t_1 I_{\mathcal{H}})^{-1} - (A_0 + t_1 I_{\mathcal{H}})^{-1}\big](A_0 + t_1 I_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1},\end{aligned} \tag{2.54}$$

one obtains

$$\begin{aligned}&\overline{(A - zI_{\mathcal{H}})^{1/2}\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big](A - zI_{\mathcal{H}})^{1/2}}\\
&\quad = \big[(A - zI_{\mathcal{H}})^{1/2}(A + t_1 I_{\mathcal{H}})^{-1/2}\big]\big[(A + t_1 I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1}\big]\\
&\qquad \times \mathrm{cl}\big\{(A + t_1 I_{\mathcal{H}})^{1/2}\big[(A + t_1 I_{\mathcal{H}})^{-1} - (A_0 + t_1 I_{\mathcal{H}})^{-1}\big](A + t_1 I_{\mathcal{H}})^{1/2}\\
&\qquad \times (A + t_1 I_{\mathcal{H}})^{-1/2}(A_0 + t_1 I_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}\big\}\\
&\quad = \big[(A - zI_{\mathcal{H}})^{1/2}(A + t_1 I_{\mathcal{H}})^{-1/2}\big]\big[(A + t_1 I_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1}\big]\\
&\qquad \times \overline{(A + t_1 I_{\mathcal{H}})^{1/2}\big[(A + t_1 I_{\mathcal{H}})^{-1} - (A_0 + t_1 I_{\mathcal{H}})^{-1}\big](A + t_1 I_{\mathcal{H}})^{1/2}}\\
&\qquad \times \big\{(A - zI_{\mathcal{H}})^{1/2}(A + t_1 I_{\mathcal{H}})^{-1/2}\\
&\qquad\quad + (z + t)(A + t_1 I_{\mathcal{H}})^{-1/2}(A - zI_{\mathcal{H}})^{-1/2}\big[(A^* - \overline{z}I_{\mathcal{H}})^{1/2}(A_0^* - \overline{z}I_{\mathcal{H}})^{-1/2}\big]^*\big\},\end{aligned} \tag{2.55}$$

where we employed the identity

$$(A_0 + t_1 I_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1} = I_{\mathcal{H}} + (z + t_1)(A_0 - zI_{\mathcal{H}})^{-1} \tag{2.56}$$

and used the symbol $\mathrm{cl}\{\dots\}$ to denote the operator closure (in addition to our usual bar symbol) as the latter extends over two lines. By Lemmas 2.6 and 2.7, all square brackets $[\cdots]$ in (2.55) lie in $\mathcal{B}(\mathcal{H})$. Thus, the trace class property in assumption (2.32) proves that in (2.53).

Finally, the analyticity statements in (2.46) (see also the one in (2.51)) employed in (2.55) prove the $\mathcal{B}_1(\mathcal{H})$-analyticity of the operator in (2.53). $\square$

Theorem 2.8. *Assume that A and A_0 satisfy Hypothesis 2.4. Then*

$$\begin{aligned}&-\frac{d}{dz}\ln\Big(\det_{\mathcal{H}}\Big(\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\Big)\Big)\\ &\quad = \mathrm{tr}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big),\end{aligned} \tag{2.57}$$

for all $z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$ such that $\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}$ is boundedly invertible.

Proof. Let $z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$. We note that by (2.46) one has

$$\begin{aligned}&\overline{(A - zI_{\mathcal{H}})^{1/2}\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big](A - zI_{\mathcal{H}})^{1/2}}\\
&\quad = I_{\mathcal{H}} - \overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\\
&\quad = I_{\mathcal{H}} - \big[(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1/2}\big]\big[(A^* - \overline{z}I_{\mathcal{H}})^{1/2}(A_0^* - \overline{z}I_{\mathcal{H}})^{-1/2}\big]^*\end{aligned} \tag{2.58}$$

and hence $\det_{\mathcal{H}}\big(\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big)$ is well-defined.

Next, we consider

$$T_1(z) = (A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1/2}, \quad z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big), \tag{2.59}$$

and compute for $\varepsilon \in \mathbb{C}\backslash\{0\}$, $|\varepsilon|$ sufficiently small such that $z, z+\varepsilon \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big)$,

$$\begin{aligned}&[T_1(z + \varepsilon) - T_1(z)]\\ &\quad = (A - (z + \varepsilon)I_{\mathcal{H}})(A - (z + \varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z + \varepsilon)I_{\mathcal{H}})^{-1/2}\end{aligned}$$

$$
\begin{aligned}
&\quad - (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}(A_0 - zI_{\mathcal{H}})^{-1/2} \\
&= (A - (z+\varepsilon)I_{\mathcal{H}})(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad - (A - zI_{\mathcal{H}})(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad + (A - zI_{\mathcal{H}})(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad - (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}(A_0 - zI_{\mathcal{H}})^{-1/2} \\
&= -\varepsilon(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad + (A - zI_{\mathcal{H}})(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad - (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad + (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad - (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}(A_0 - zI_{\mathcal{H}})^{-1/2} \\
&= -\varepsilon(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\quad + (A - zI_{\mathcal{H}})\big[(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} - (A - zI_{\mathcal{H}})^{-1/2}\big] \\
&\qquad \times (A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \qquad (2.60) \\
&\quad + (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}\big[(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} - (A_0 - zI_{\mathcal{H}})^{-1/2}\big].
\end{aligned}
$$

Using

$$
\begin{aligned}
&\big[(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} - (A - zI_{\mathcal{H}})^{-1/2}\big] \\
&\quad = \frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}\big[(A + (t-z-\varepsilon)I_{\mathcal{H}})^{-1} - (A + (t-z)I_{\mathcal{H}})^{-1}\big] \\
&\quad = \frac{\varepsilon}{\pi}\int_0^\infty dt\, t^{-1/2}(A + (t-z-\varepsilon)I_{\mathcal{H}})^{-1}(A + (t-z)I_{\mathcal{H}})^{-1} \qquad (2.61)
\end{aligned}
$$

in (2.60) yields

$$
\begin{aligned}
&\frac{1}{\varepsilon}[T_1(z+\varepsilon) - T_1(z)] = -(A - (z+\varepsilon)I_{\mathcal{H}})^{-1/2}(A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\qquad + (A - zI_{\mathcal{H}})\bigg[\frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A + (t-z-\varepsilon)I_{\mathcal{H}})^{-1}(A + (t-z)I_{\mathcal{H}})^{-1}\bigg] \\
&\qquad\quad \times (A_0 - (z+\varepsilon)I_{\mathcal{H}})^{-1/2} \\
&\qquad + (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2} \\
&\qquad\quad \times \bigg[\frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A_0 + (t-z-\varepsilon)I_{\mathcal{H}})^{-1}(A_0 + (t-z)I_{\mathcal{H}})^{-1}\bigg] \\
&\underset{\varepsilon\to 0}{\longrightarrow} -(A - zI_{\mathcal{H}})^{-1/2}(A_0 - zI_{\mathcal{H}})^{-1/2} \\
&\qquad + (A - zI_{\mathcal{H}})\bigg[\frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A + (t-z)I_{\mathcal{H}})^{-2}\bigg](A_0 - zI_{\mathcal{H}})^{-1/2} \\
&\qquad + (A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-1/2}\bigg[\frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A_0 + (t-z)I_{\mathcal{H}})^{-2}\bigg] \\
&= -(A - zI_{\mathcal{H}})^{-1/2}(A_0 - zI_{\mathcal{H}})^{-1/2} \\
&\quad + \frac{1}{2}(A - zI_{\mathcal{H}})(A - zI_{\mathcal{H}})^{-3/2}(A_0 - zI_{\mathcal{H}})^{-1/2}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{2}(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-3/2}\\
&=-\frac{1}{2}(A-zI_{\mathcal{H}})^{-1/2}(A_0-zI_{\mathcal{H}})^{-1/2}\\
&\quad+\frac{1}{2}(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-3/2},
\end{aligned}
\tag{2.62}
$$

where the limit $\varepsilon \to 0$ is valid in the $\mathcal{B}(\mathcal{H})$-norm. Here we used (cf. (2.21) applied to $\alpha = 3/2$ and A replaced by $(A - zI_{\mathcal{H}})$)

$$
\frac{1}{\pi}\int_0^\infty dt\, t^{-1/2}(A+(t-z)I_{\mathcal{H}})^{-2} = \frac{1}{2}(A-zI_{\mathcal{H}})^{-3/2}, \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big). \tag{2.63}
$$

Thus,

$$
\begin{aligned}
T_1'(z) = -\frac{1}{2}(A-zI_{\mathcal{H}})^{-1/2}(A_0-zI_{\mathcal{H}})^{-1/2} + \frac{1}{2}(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-3/2},&\\
z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big).&
\end{aligned}
\tag{2.64}
$$

Similarly, introducing

$$
T_2(z) = \big[(A^*-\overline{z}I_{\mathcal{H}})^{1/2}(A_0^*-\overline{z}I_{\mathcal{H}})^{-1/2}\big]^*, \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big), \tag{2.65}
$$

one obtains

$$
\begin{aligned}
T_2'(z) = &-\frac{1}{2}\big[(A^*-\overline{z}I_{\mathcal{H}})^{-1/2}(A_0-zI_{\mathcal{H}})^{-1/2}\big]^*\\
&+\frac{1}{2}\big[(A^*-\overline{z}I_{\mathcal{H}})^{1/2}(A_0^*-\overline{z}I_{\mathcal{H}})^{-3/2}\big]^*, \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big).
\end{aligned}
\tag{2.66}
$$

Consequently, one computes

$$
\begin{aligned}
&\frac{d}{dz}\Big[\overline{(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-1}(A-zI_{\mathcal{H}})^{1/2}}\Big]\\
&\quad= [T_1(z)T_2(z)]' = T_1'(z)T_2(z) + T_1(z)T_2'(z)\\
&\quad= \Big[-\frac{1}{2}(A-zI_{\mathcal{H}})^{-1/2}(A_0-zI_{\mathcal{H}})^{-1/2} + \frac{1}{2}(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-3/2}\Big]\\
&\qquad\times\big[(A^*-\overline{z}I_{\mathcal{H}})^{1/2}(A_0^*-\overline{z}I_{\mathcal{H}})^{-1/2}\big]^*\\
&\qquad+\big[(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-1/2}\big]\Big[-\frac{1}{2}\big[(A^*-\overline{z}I_{\mathcal{H}})^{-1/2}(A_0^*-\overline{z}I_{\mathcal{H}})^{-1/2}\big]^*\\
&\qquad\quad+\frac{1}{2}\big[(A^*-\overline{z}I_{\mathcal{H}})^{1/2}(A_0^*-\overline{z}I_{\mathcal{H}})^{-3/2}\big]^*\Big]\\
&\quad= -\frac{1}{2}\overline{(A-zI_{\mathcal{H}})^{-1/2}(A_0-zI_{\mathcal{H}})^{-1}(A-zI_{\mathcal{H}})^{1/2}}\\
&\qquad-\frac{1}{2}\overline{(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-1}(A-zI_{\mathcal{H}})^{-1/2}}\\
&\qquad+\overline{(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-2}(A-zI_{\mathcal{H}})^{1/2}}, \quad z \in \mathbb{C}\backslash\big(\overline{-t_0+S_{\omega_0}}\big).
\end{aligned}
\tag{2.67}
$$

Due to the $\mathcal{B}_1(\mathcal{H})$-analyticity of the left-hand side of (2.58) according to Lemma 2.7, one can apply (2.1), and using the result (2.67) one finally obtains

$$
\begin{aligned}
&-\frac{d}{dz}\ln\Big(\det{}_{\mathcal{H}}\Big(\overline{(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-1}(A-zI_{\mathcal{H}})^{1/2}}\Big)\Big)\\
&\quad= -\operatorname{tr}_{\mathcal{H}}\Big(\big\{\overline{(A-zI_{\mathcal{H}})^{1/2}(A_0-zI_{\mathcal{H}})^{-1}(A-zI_{\mathcal{H}})^{1/2}}\big\}^{-1}
\end{aligned}
$$

$$
\begin{aligned}
&\quad \times \big[\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big]'\Big) \\
&= \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big(\big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}^{-1} \\
&\quad \times \big\{\overline{(A - zI_{\mathcal{H}})^{-1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}} \\
&\qquad - 2\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-2}(A - zI_{\mathcal{H}})^{1/2}} \\
&\qquad + \overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{-1/2}}\big\}\Big) \\
&= \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big(\big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}^{-1} \\
&\quad \times (A - zI_{\mathcal{H}})^{1/2}\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big] \\
&\quad \times \overline{(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\Big) \\
&\quad + \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big(\big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}^{-1} \\
&\qquad \times (A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1} \\
&\qquad \times \overline{\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big](A - zI_{\mathcal{H}})^{1/2}}\Big) \\
&= \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big(\big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}^{-1} \\
&\quad \times (A - zI_{\mathcal{H}})^{1/2}\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big] \\
&\quad \times (A - zI_{\mathcal{H}})^{-1/2}\big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}\Big) \\
&\quad + \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big(\big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}^{-1} \\
&\qquad \times \big\{\overline{(A - zI_{\mathcal{H}})^{1/2}(A_0 - zI_{\mathcal{H}})^{-1}(A - zI_{\mathcal{H}})^{1/2}}\big\}(A - zI_{\mathcal{H}})^{-1/2} \\
&\qquad \times \overline{\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big](A - zI_{\mathcal{H}})^{1/2}}\Big) \\
&= \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big((A - zI_{\mathcal{H}})^{1/2}\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big](A - zI_{\mathcal{H}})^{-1/2}\Big) \\
&\quad + \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\Big((A - zI_{\mathcal{H}})^{-1/2}\overline{\big[(A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big](A - zI_{\mathcal{H}})^{1/2}}\Big) \\
&= \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big) + \frac{1}{2}\operatorname{tr}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big) \\
&= \operatorname{tr}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})^{-1} - (A_0 - zI_{\mathcal{H}})^{-1}\big), \quad z \in \mathbb{C}\backslash\big(\overline{-t_0 + S_{\omega_0}}\big). \qquad (2.68)
\end{aligned}
$$

Here we repeatedly used cyclicity of the trace. □

Remark 2.9. (i) Extensions of the standard perturbation determinant

$$\det{}_{\mathcal{H}}\big((A - zI_{\mathcal{H}})(A_0 - zI_{\mathcal{H}})^{-1}\big) = \det{}_{\mathcal{H}}\big(I_{\mathcal{H}} + (A - A_0)(A_0 - zI_{\mathcal{H}})^{-1}\big) \qquad (2.69)$$

to certain symmetrized (sometimes called, modified) versions involving factorizations of $A - A_0$ have been considered in [46] and [72, Sect. 8.1.4]. However, Theorem 2.8 appears to be of a more general nature and of independent interest.
(ii) We emphasize the general nature of the hypotheses on A, A_0 in Theorem 2.8. In particular, it covers the frequently encountered special case of self-adjoint operators A, A_0 with A_0 bounded from below and A a quadratic form perturbation of A_0 with relative bound strictly less than one, in addition to the trace class requirement

(2.32). In this case one has $\operatorname{dom}\big(|A_0|^{1/2}\big) = \operatorname{dom}\big(|A|^{1/2}\big)$. Actually, Theorem 2.8 permits the more general situation where the latter equality of form domains is replaced by $\operatorname{dom}\big(|A_0|^{1/2}\big) \subseteq \operatorname{dom}\big(|A|^{1/2}\big)$. The latter fact will have to be used in our application to one-dimensional Schrödinger operators on a compact interval in Section 4 in the case where the separated boundary conditions involve a Dirichlet boundary condition at one or both interval endpoints.
(iii) Going beyond item $(VIII)$, we also note that Theorem 2.8 applies when A, A_0 are (Dunford) spectral operators of scalar type [20, Ch. XVIII] (in the sense that their resolvent is similar to the resolvent of a self-adjoint operator) with real spectrum bounded from below.

3. Boundary Data Maps and Their Basic Properties

This section is devoted to a brief review of boundary data maps as recently introduced in [14]. The results taken from [14] are presented without proof (for detailed proofs and for an extensive bibliography we refer to [14]). We will also present a few new results of boundary data maps in this section (and then of course supply proofs).

Taking $R > 0$, and fixing $\theta_0, \theta_R \in S_{2\pi}$, with $S_{2\pi}$ the strip

$$S_{2\pi} = \{z \in \mathbb{C} \,|\, 0 \leq \operatorname{Re}(z) < 2\pi\}, \tag{3.1}$$

we introduce the linear map $\gamma_{\theta_0,\theta_R}$, the trace map associated with the boundary $\{0, R\}$ of $(0, R)$ and the parameters θ_0, θ_R, by

$$\gamma_{\theta_0,\theta_R} \colon \begin{cases} C^1([0,R]) \to \mathbb{C}^2, \\ u \mapsto \begin{bmatrix} \cos(\theta_0)u(0) + \sin(\theta_0)u'(0) \\ \cos(\theta_R)u(R) - \sin(\theta_R)u'(R) \end{bmatrix}, \end{cases} \qquad \theta_0, \theta_R \in S_{2\pi}, \tag{3.2}$$

where "prime" denotes d/dx. We note, in particular, that the Dirichlet trace γ_D, and the Neumnann trace γ_N (in connection with the outward pointing unit normal vector at $\partial(0, R) = \{0, R\}$), are given by

$$\gamma_D = \gamma_{0,0} = -\gamma_{\pi,\pi}, \quad \gamma_N = \gamma_{3\pi/2,3\pi/2} = -\gamma_{\pi/2,\pi/2}. \tag{3.3}$$

Next, assuming

$$V \in L^1((0,R); dx), \tag{3.4}$$

we introduce the following family of densely defined closed linear operators H_{θ_0,θ_R} in $L^2((0, R); dx)$,

$$\begin{aligned} &H_{\theta_0,\theta_R} f = -f'' + Vf, \quad \theta_0, \theta_R \in S_{2\pi}, \\ &f \in \operatorname{dom}(H_{\theta_0,\theta_R}) = \big\{g \in L^2((0,R); dx) \,\big|\, g, g' \in AC([0,R]);\ \gamma_{\theta_0,\theta_R}(g) = 0; \\ &\hspace{6cm} (-g'' + Vg) \in L^2((0,R); dx)\big\}. \end{aligned} \tag{3.5}$$

Here $AC([0, R])$ denotes the set of absolutely continuous functions on $[0, R]$. We remark that V is not assumed to be real-valued in this section. It is well-known that the spectrum of H_{θ_0,θ_R}, $\sigma(H_{\theta_0,\theta_R})$ is purely discrete,

$$\sigma(H_{\theta_0,\theta_R}) = \sigma_{\mathrm{d}}(H_{\theta_0,\theta_R}), \quad \theta_0, \theta_R \in S_{2\pi}. \tag{3.6}$$

In addition, the resolvent of H_{θ_0,θ_R} is a Hilbert–Schmidt operator in $L^2((0,R);dx)$ and the eigenvalues $E_{\theta_0,\theta_R,n}$ of H_{θ_0,θ_R}, in the case of the separated boundary conditions at hand, are of the form

$$E_{\theta_0,\theta_R,n} \underset{n\to\infty}{=} [(n\pi/R)+(a_n/n)]^2 \text{ with } a_n\in\ell^\infty(\mathbb{N}), \tag{3.7}$$

as shown in [55, Lemma 1.3.3]. Moreover, H_{θ_0,θ_R} is known to be m-sectorial (cf. [21, Sect. III.6], [39, Sect. VI.2.4]).

One notices that

$$\gamma_{(\theta_0+\pi)\bmod(2\pi),(\theta_R+\pi)\bmod(2\pi)} = -\gamma_{\theta_0,\theta_R}, \quad \theta_0,\theta_R\in S_{2\pi}, \tag{3.8}$$

and, on the other hand,

$$H_{(\theta_0+\pi)\bmod(2\pi),(\theta_R+\pi)\bmod(2\pi)} = H_{\theta_0,\theta_R}, \quad \theta_0,\theta_R\in S_{2\pi}, \tag{3.9}$$

hence it suffices to consider $\theta_0,\theta_R\in S_\pi=\{z\in\mathbb{C}\,|\,0\le \mathrm{Re}(z)<\pi\}$ rather than $\theta_0,\theta_R\in S_{2\pi}$ in connection with H_{θ_0,θ_R}, but for simplicity of notation we will keep using the strip $S_{2\pi}$ throughout this manuscript.

The adjoint of H_{θ_0,θ_R} is given by

$$\begin{aligned}
&(H_{\theta_0,\theta_R})^*f = -f''+\overline{V}f, \quad \theta_0,\theta_R\in S_{2\pi},\\
&f\in\mathrm{dom}\big((H_{\theta_0,\theta_R})^*\big) = \big\{g\in L^2((0,R);dx)\,\big|\, g,g'\in AC([0,R]);\ \gamma_{\overline{\theta_0},\overline{\theta_R}}(g)=0;\\
&\hspace{6cm} (-g''+\overline{V}g)\in L^2((0,R);dx)\big\}.
\end{aligned} \tag{3.10}$$

Having described the operator H_{θ_0,θ_R} is some detail, still assuming (3.4), we now briefly recall the corresponding closed, sectorial, and densely defined sequilinear form, denoted by $Q_{H_{\theta_0,\theta_R}}$, associated with H_{θ_0,θ_R} (cf. [39, p. 312, 321, 327–328]):

$$\begin{aligned}
Q_{H_{\theta_0,\theta_R}}(f,g) &= \int_0^R dx\big[\overline{f'(x)}g'(x)+V(x)\overline{f(x)}g(x)\big]\\
&\quad -\cot(\theta_0)\overline{f(0)}g(0)-\cot(\theta_R)\overline{f(R)}g(R),
\end{aligned} \tag{3.11}$$

$$\begin{aligned}
f,g\in\mathrm{dom}(Q_{H_{\theta_0,\theta_R}}) &= H^1((0,R))\\
&= \big\{h\in L^2((0,R);dx)\,|\,h\in AC([0,R]);\ h'\in L^2((0,R);dx)\big\},\\
&\hspace{5cm}\theta_0,\theta_R\in S_{2\pi}\backslash\{0,\pi\},
\end{aligned}$$

$$Q_{H_{0,\theta_R}}(f,g) = \int_0^R dx\big[\overline{f'(x)}g'(x)+V(x)\overline{f(x)}g(x)\big]-\cot(\theta_R)\overline{f(R)}g(R), \tag{3.12}$$

$$\begin{aligned}
&f,g\in\mathrm{dom}(Q_{H_{0,\theta_R}})\\
&\quad = \big\{h\in L^2((0,R);dx)\,|\,h\in AC([0,R]);\ h(0)=0;\ h'\in L^2((0,R);dx)\big\},\\
&\hspace{8cm}\theta_R\in S_{2\pi}\backslash\{0,\pi\},
\end{aligned}$$

$$Q_{H_{\theta_0,0}}(f,g) = \int_0^R dx\big[\overline{f'(x)}g'(x)+V(x)\overline{f(x)}g(x)\big]-\cot(\theta_0)\overline{f(0)}g(0), \tag{3.13}$$

$$\begin{aligned}
&f,g\in\mathrm{dom}(Q_{H_{\theta_0,0}})\\
&\quad = \big\{h\in L^2((0,R);dx)\,|\,h\in AC([0,R]);\ h(R)=0;\ h'\in L^2((0,R);dx)\big\},\\
&\hspace{8cm}\theta_0\in S_{2\pi}\backslash\{0,\pi\},
\end{aligned}$$

$$Q_{H_{0,0}}(f,g) = \int_0^R dx\big[\overline{f'(x)}g'(x)+V(x)\overline{f(x)}g(x)\big], \tag{3.14}$$

$$\begin{aligned} f,g \in \operatorname{dom}(Q_{H_{0,0}}) &= \operatorname{dom}\big(|H_{0,0}|^{1/2}\big) = H_0^1((0,R)) \\ &= \big\{h \in L^2((0,R);dx) \,|\, h \in AC([0,R]);\ h(0)=0,\ h(R)=0; \\ &\qquad\qquad\qquad\qquad\qquad h' \in L^2((0,R);dx)\big\}. \end{aligned}$$

Next, we recall the following elementary, yet fundamental, fact:

Lemma 3.1. *Suppose that $V \in L^1((0,R);dx)$, fix $\theta_0, \theta_R \in S_{2\pi}$, and assume that $z \in \mathbb{C}\backslash\sigma(H_{\theta_0,\theta_R})$. Then the boundary value problem given by*

$$-u'' + Vu = zu, \quad u, u' \in AC([0,R]), \tag{3.15}$$

$$\gamma_{\theta_0,\theta_R}(u) = \begin{bmatrix} c_0 \\ c_R \end{bmatrix} \in \mathbb{C}^2, \tag{3.16}$$

has a unique solution $u(z,\cdot) = u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))$ for each $c_0, c_R \in \mathbb{C}$.

Assuming $z \in \rho(H_{\theta_0,\theta_R})$, a basis for the solutions of (3.15) is given by

$$\begin{aligned} u_{-,\theta_0}(z,\cdot) &= u(z,\cdot\,;(\theta_0,0),(0,1)), \\ u_{+,\theta_R}(z,\cdot) &= u(z,\cdot\,;(0,1),(\theta_R,0)). \end{aligned} \tag{3.17}$$

Explicitly, one then has

$$u_{-,\theta_0}(z,R) = 1, \quad \cos(\theta_0)u_{-,\theta_0}(z,0) + \sin(\theta_0)u'_{-,\theta_0}(z,0) = 0, \tag{3.18}$$

$$u_{+,\theta_R}(z,0) = 1, \quad \cos(\theta_R)u_{+,\theta_R}(z,R) - \sin(\theta_R)u'_{+,\theta_R}(z,R) = 0. \tag{3.19}$$

Recalling the Wronskian of two functions f and g,

$$W(f,g)(x) = f(x)g'(x) - f'(x)g(x), \quad f,g \in C^1([0,R]), \tag{3.20}$$

one then computes

$$W(u_{+,\theta_R}(z,\cdot), u_{-,\theta_0}(z,\cdot)) = u'_{-,\theta_0}(z,0) - u'_{+,\theta_R}(z,0)u_{-,\theta_0}(z,0) \tag{3.21}$$

$$= u_{+,\theta_R}(z,R)u'_{-,\theta_0}(z,R) - u'_{+,\theta_R}(z,R). \tag{3.22}$$

To each boundary value problem (3.15), (3.16), we now associate a family of *general boundary data maps*, $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) : \mathbb{C}^2 \to \mathbb{C}^2$, for $\theta_0, \theta_R, \theta_0', \theta_R' \in S_{2\pi}$, where

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\begin{bmatrix} c_0 \\ c_R \end{bmatrix} &= \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\big(\gamma_{\theta_0,\theta_R}(u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R)))\big) \\ &= \gamma_{\theta_0',\theta_R'}(u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))). \end{aligned} \tag{3.23}$$

With $u(z,\cdot) = u(z,\cdot\,;(\theta_0,c_0),(\theta_R,c_R))$, then $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ can be represented as a 2×2 complex matrix, where

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\begin{bmatrix} c_0 \\ c_R \end{bmatrix} &= \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\begin{bmatrix} \cos(\theta_0)u(z,0) + \sin(\theta_0)u'(z,0) \\ \cos(\theta_R)u(z,R) - \sin(\theta_R)u'(z,R) \end{bmatrix} \\ &= \begin{bmatrix} \cos(\theta_0')u(z,0) + \sin(\theta_0')u'(z,0) \\ \cos(\theta_R')u(z,R) - \sin(\theta_R')u'(z,R) \end{bmatrix}. \end{aligned} \tag{3.24}$$

One can show that $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}$ is well-defined for $z \in \rho(H_{\theta_0,\theta_R})$, that is, it is invariant with respect to a change of basis of solutions of (3.15) (cf. [14, Theorem 2.3]). Moreover, one has the following facts: Let $\theta_0, \theta_R, \theta_0', \theta_R', \theta_0'', \theta_R'' \in S_{2\pi}$. Then, with I_2 denoting the identity matrix in $\mathbb{C}^2$,

$$\Lambda_{\theta_0,\theta_R}^{\theta_0,\theta_R}(z) = I_2, \quad z \in \rho(H_{\theta_0,\theta_R}), \tag{3.25}$$

$$\Lambda_{\theta_0',\theta_R'}^{\theta_0'',\theta_R''}(z)\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) = \Lambda_{\theta_0,\theta_R}^{\theta_0'',\theta_R''}(z), \quad z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{\theta_0',\theta_R'}), \tag{3.26}$$

$$\Lambda_{\theta_0',\theta_R'}^{\theta_0,\theta_R}(z) = \Big[\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big]^{-1}, \quad z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{\theta_0',\theta_R'}). \tag{3.27}$$

Remark 3.2. Even though $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}$ is invariant with respect to a change of basis for the solutions of (3.15), the representation of $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}$ with respect to a specific basis can be simplified considerably with an appropriate choice of basis. For example, by choosing the basis given in (3.17), and by letting $\psi_1(z,\cdot) = u_{+,\theta_R}(z,\cdot) = u(z,\cdot\,;(0,1),(\theta_R,0))$, and $\psi_2(z,\cdot) = u_{-,\theta_0}(z,\cdot) = u(z,\cdot\,;(\theta_0,0),(0,1))$, one obtains using this basis,

$$\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) = \Big[\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)_{j,k}\Big]_{1\le j,k\le 2}, \quad z \in \rho(H_{\theta_0,\theta_R}), \tag{3.28}$$

$$\begin{aligned}
\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)_{1,1} &= \frac{\cos(\theta_0') + \sin(\theta_0')u_{+,\theta_R}'(z,0)}{\cos(\theta_0) + \sin(\theta_0)u_{+,\theta_R}'(z,0)}, \\
\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)_{1,2} &= \frac{\cos(\theta_0')u_{-,\theta_0}(z,0) + \sin(\theta_0')u_{-,\theta_0}'(z,0)}{\cos(\theta_R) - \sin(\theta_R)u_{-,\theta_0}'(z,R)}, \\
\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)_{2,1} &= \frac{\cos(\theta_R')u_{+,\theta_R}(z,R) - \sin(\theta_R')u_{+,\theta_R}'(z,R)}{\cos(\theta_0) + \sin(\theta_0)u_{+,\theta_R}'(z,0)}, \\
\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)_{2,2} &= \frac{\cos(\theta_R') - \sin(\theta_R')u_{-,\theta_0}'(z,R)}{\cos(\theta_R) - \sin(\theta_R)u_{-,\theta_0}'(z,R)}.
\end{aligned} \tag{3.29}$$

In particular, by (3.18) and (3.19),

$$\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0,\theta_R'}(z)\Big)_{1,2} = 0, \quad \Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R}(z)\Big)_{2,1} = 0. \tag{3.30}$$

Remark 3.3. We note that $\Lambda_{0,0}^{\frac{\pi}{2},\frac{\pi}{2}}(z)$ represents the *Dirichlet-to-Neumann map*, $\Lambda_{D,N}(z)$, for the boundary value problem (3.15), (3.16); that is, when $\theta_0 = \theta_R = 0$, $\theta_0' = \theta_R' = \pi/2$, then (3.24) becomes

$$\Lambda_{D,N}(z)\begin{bmatrix} u(z,0) \\ u(z,R) \end{bmatrix} = \Lambda_{0,0}^{\frac{\pi}{2},\frac{\pi}{2}}(z)\begin{bmatrix} u(z,0) \\ u(z,R) \end{bmatrix} = \begin{bmatrix} u'(z,0) \\ -u'(z,R) \end{bmatrix}, \quad z \in \rho(H_{\theta_0,\theta_R}), \tag{3.31}$$

with $u(z,\cdot) = u(z,\cdot\,;(0,c_0),(0,c_R))$, $u(z,0) = c_0$, $u(z,R) = c_R$. The Dirichlet-to-Neumann map in the case $V = 0$ has recently been considered in [63, Example 5.1]. The Neumann-to-Dirichlet map $\Lambda_{N,D}(z) = \Lambda_{\pi/2,\pi/2}^{\pi,\pi}(z) = -[\Lambda_{D,N}(z)]^{-1}$ in the case $V = 0$ has earlier been computed in [17, Example 4.1]. We also refer to [8], [12], [16] in the intimately related context of Q and M-functions.

We continue with an elementary result needed in the proof of Lemma 3.4, but first we introduce a convenient basis of solutions associated with the Schrödinger equation (3.15): Fix $z \in \mathbb{C}$ and let $\theta(z,\cdot), \theta'(z,\cdot), \phi(z,\cdot), \phi'(z,\cdot) \in AC([0,R])$, and such that $\theta(z,\cdot)$ and $\phi(z,\cdot)$ are solutions of

$$-u'' + Vu = zu, \tag{3.32}$$

uniquely determined by their initial values at $x = 0$,

$$\theta(z,0) = \phi'(z,0) = 1, \quad \theta'(z,0) = \phi(z,0) = 0. \tag{3.33}$$

In particular, $\theta(z,\cdot)$ and $\phi(z,\cdot)$ are entire with respect to z. Introducing

$$\psi(z,\cdot) = A\theta(z,\cdot) + B\phi(z,\cdot), \quad A, B \in \mathbb{C}, \tag{3.34}$$

it follows that

$$\gamma_{\theta_0,\theta_R}(\psi) = \begin{bmatrix} \cos(\theta_0)\psi(z,0) + \sin(\theta_0)\psi'(z,0) \\ \cos(\theta_R)\psi(z,R) - \sin(\theta_R)\psi'(z,R) \end{bmatrix} = 0 \in \mathbb{C}^2 \tag{3.35}$$

is equivalent to

$$\begin{aligned} 0 &= \begin{bmatrix} \cos(\theta_0) & \sin(\theta_0) \\ \cos(\theta_R)\theta(z,R) - \sin(\theta_R)\theta'(z,R) & \cos(\theta_R)\phi(z,R) - \sin(\theta_R)\phi'(z,R) \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} \\ &= \mathcal{U}(z,R,\theta_0,\theta_R) \begin{bmatrix} A \\ B \end{bmatrix}. \end{aligned} \tag{3.36}$$

Consequently, introducing the determinant Δ defined by

$$\Delta(z,R,\theta_0,\theta_R) = \det\big(\mathcal{U}(z,R,\theta_0,\theta_R)\big), \tag{3.37}$$

one concludes that

$$z_0 \text{ is an eigenvalue of } H_{\theta_0,\theta_R} \Longleftrightarrow z_0 \text{ is a zero of the determinant } \Delta(\cdot,R,\theta_0,\theta_R). \tag{3.38}$$

Moreover, Δ is an entire function with respect to z, and an explicit computation reveals that

$$\begin{aligned} \Delta(z,R,\theta_0,\theta_R) = \cos(\theta_0)\cos(\theta_R)\phi(z,R) - \cos(\theta_0)\sin(\theta_R)\phi'(z,R) \\ - \sin(\theta_0)\cos(\theta_R)\theta(z,R) + \sin(\theta_0)\sin(\theta_R)\theta'(z,R). \end{aligned} \tag{3.39}$$

In addition, we point out that the function Δ is closely related to the usual Wronskian of two solution $u_{\pm,\theta_0,\theta_R}$ of (3.32) satisfying the boundary conditions

$$\cos(\theta_0)u_{+,\theta_0,\theta_R}(z,0) + \sin(\theta_0)u'_{+,\theta_0,\theta_R}(z,0) = 1, \tag{3.40}$$

$$\cos(\theta_R)u_{+,\theta_0,\theta_R}(z,R) - \sin(\theta_R)u'_{+,\theta_0,\theta_R}(z,R) = 0, \tag{3.41}$$

$$\cos(\theta_0)u_{-,\theta_0,\theta_R}(z,0) + \sin(\theta_0)u'_{-,\theta_0,\theta_R}(z,0) = 0, \tag{3.42}$$

$$\cos(\theta_R)u_{-,\theta_0,\theta_R}(z,R) - \sin(\theta_R)u'_{-,\theta_0,\theta_R}(z,R) = 1. \tag{3.43}$$

In vector form, these boundary conditions correspond to

$$\big[\gamma_{\theta_0,\theta_R}(u_{+,\theta_0,\theta_R}) \quad \gamma_{\theta_0,\theta_R}(u_{-,\theta_0,\theta_R})\big] = I_2. \tag{3.44}$$

Since $\gamma_{\theta_0,\theta_R}$ is a linear map, it follows from (3.34) that

$$\gamma_{\theta_0,\theta_R}(\psi) = \big[\gamma_{\theta_0,\theta_R}(\theta) \quad \gamma_{\theta_0,\theta_R}(\phi)\big] \begin{bmatrix} A \\ B \end{bmatrix}, \tag{3.45}$$

hence by (3.36)

$$\mathcal{U}(z,R,\theta_0,\theta_R) = \big[\gamma_{\theta_0,\theta_R}(\theta) \quad \gamma_{\theta_0,\theta_R}(\phi)\big]. \tag{3.46}$$

Using (3.44) and the linearity of $\gamma_{\theta_0,\theta_R}$ once again one concludes that

$$\big[u_{+,\theta_0,\theta_R}(z,x) \quad u_{-,\theta_0,\theta_R}(z,x)\big] = \big[\theta(z,x) \quad \phi(z,x)\big]\big[\gamma_{\theta_0,\theta_R}(\theta) \quad \gamma_{\theta_0,\theta_R}(\phi)\big]^{-1} \tag{3.47}$$

since both sides solve (3.32) and satisfy the same boundary condition. Thus, (3.46) and (3.47) yield

$$W(u_{+,\theta_0,\theta_R}(z,\cdot), u_{-,\theta_0,\theta_R}(z,\cdot)) = W(\theta(z,\cdot),\phi(z,\cdot))\det(\mathcal{U}(z,R,\theta_0,\theta_R)^{-1})$$

$$= \Delta(z,R,\theta_0,\theta_R)^{-1}, \tag{3.48}$$

where $W(\cdot,\cdot)$ denotes the Wronskian of two functions as introduced in (3.20).

Lemma 3.4. *Assume that $\theta_0,\theta_R,\theta_0',\theta_R' \in S_{2\pi}$, and let H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ be defined as in* (3.5)*. Then, with $\Delta(\cdot,R,\theta_0,\theta_R)$ introduced in* (3.37)*,*

$$\det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big) = \frac{\Delta(z,R,\theta_0',\theta_R')}{\Delta(z,R,\theta_0,\theta_R)}, \quad z \in \rho(H_{\theta_0,\theta_R}). \tag{3.49}$$

Proof. We recall the formula

$$\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) = \big[\gamma_{\theta_0',\theta_R'}(\theta(z,\cdot)) \quad \gamma_{\theta_0',\theta_R'}(\phi(z,\cdot))\big]\big[\gamma_{\theta_0,\theta_R}(\theta(z,\cdot)) \quad \gamma_{\theta_0,\theta_R}(\phi(z,\cdot)\big]^{-1}, \tag{3.50}$$

established in the proof of Theorem 2.3 in [14]. Since

$$\begin{aligned}
&\big[\gamma_{\theta_0,\theta_R}(\theta(z,\cdot)) \quad \gamma_{\theta_0,\theta_R}(\phi(z,\cdot)\big] \\
&\quad = \begin{pmatrix} \cos(\theta_0) & \sin(\theta_0) \\ \cos(\theta_R)\theta(z,R) - \sin(\theta_R)\theta'(z,R) & \cos(\theta_R)\phi(z,R) - \sin(\theta_R)\phi'(z,R) \end{pmatrix},
\end{aligned} \tag{3.51}$$

one verifies

$$\det_{\mathbb{C}^2}\big(\big[\gamma_{\theta_0,\theta_R}(\theta(z,\cdot)) \quad \gamma_{\theta_0,\theta_R}(\phi(z,\cdot)\big]\big) = \Delta(z,R,\theta_0,\theta_R), \quad z \in \mathbb{C}, \tag{3.52}$$

and hence (3.49). $\square$

The following asymptotic expansion results will be used in the proof of Theorem 5.3:

Lemma 3.5. *Assume that $\theta_0,\theta_R \in S_{2\pi}$, $\theta_0',\theta_R' \in S_{2\pi}\backslash\{0,\pi\}$, and let H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ be defined as in* (3.5)*. Then,*

$$\begin{aligned}
&\det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big) \\
&\underset{\substack{|z|\to\infty \\ \operatorname{Im}(z^{1/2})>0}}{=} \begin{cases} \frac{\sin(\theta_0')\sin(\theta_R')}{\sin(\theta_0)\sin(\theta_R)} + O(|z|^{-1/2}), & \theta_0,\theta_R \in S_{2\pi}\backslash\{0,\pi\}, \\ -\frac{\sin(\theta_0')\sin(\theta_R')}{\sin(\theta_R)}|z|^{1/2} + O(1), & \theta_0 = 0,\ \theta_R \in S_{2\pi}\backslash\{0,\pi\}, \\ -\frac{\sin(\theta_0')\sin(\theta_R')}{\sin(\theta_0)}|z|^{1/2} + O(1), & \theta_0 \in S_{2\pi}\backslash\{0,\pi\},\ \theta_R = 0, \\ \sin(\theta_0')\sin(\theta_R')|z| + O(|z|^{1/2}), & \theta_0 = \theta_R = 0. \end{cases}
\end{aligned} \tag{3.53}$$

Proof. The standard Volterra integral equations

$$\theta(z,x) = \cos(z^{1/2}x) + \int_0^x dx'\, \frac{\sin(z^{1/2}(x-x'))}{z^{1/2}} V(x')\theta(z,x'), \tag{3.54}$$

$$\phi(z,x) = \frac{\sin(z^{1/2}x)}{z^{1/2}} + \int_0^x dx'\, \frac{\sin(z^{1/2}(x-x'))}{z^{1/2}} V(x')\phi(z,x'), \tag{3.55}$$

$$z \in \mathbb{C},\ \operatorname{Im}(z^{1/2}) \geq 0,\ x \in [0,R],$$

readily imply that

$$
\begin{aligned}
\theta(z,x) &\underset{|z|\to\infty}{=} \cos(z^{1/2}x) + O\Big(|z|^{-1/2}e^{\mathrm{Im}(z^{1/2})x}\Big),\\
\theta'(z,x) &\underset{|z|\to\infty}{=} -z^{1/2}\sin(z^{1/2}x) + O\Big(e^{\mathrm{Im}(z^{1/2})x}\Big),\\
\phi(z,x) &\underset{|z|\to\infty}{=} \frac{\sin(z^{1/2}x)}{z^{1/2}} + O\Big(|z|^{-1}e^{\mathrm{Im}(z^{1/2})x}\Big),\\
\phi'(z,x) &\underset{|z|\to\infty}{=} \cos(z^{1/2}x) + O\Big(|z|^{-1/2}e^{\mathrm{Im}(z^{1/2})x}\Big).
\end{aligned} \tag{3.56}
$$

An insertion of (3.56) into (3.39) then yields

$$
\Delta(z,R,\theta_0,\theta_R) \underset{\substack{|z|\to\infty\\ \mathrm{Im}(z^{1/2})>0}}{=} \begin{cases}
2^{-1}\sin(\theta_0)\sin(\theta_R)|z|^{1/2}e^{\mathrm{Im}(z^{1/2})} + O\Big(e^{\mathrm{Im}(z^{1/2}R)}\Big),\\
\hfill \theta_0,\theta_R\in S_{2\pi}\backslash\{0,\pi\},\\
-2^{-1}\sin(\theta_R)e^{\mathrm{Im}(z^{1/2})} + O\Big(|z|^{-1/2}e^{\mathrm{Im}(z^{1/2}R)}\Big),\\
\hfill \theta_0=0,\ \theta_R\in S_{2\pi}\backslash\{0,\pi\},\\
-2^{-1}\sin(\theta_0)e^{\mathrm{Im}(z^{1/2})} + O\Big(|z|^{-1/2}e^{\mathrm{Im}(z^{1/2}R)}\Big),\\
\hfill \theta_0\in S_{2\pi}\backslash\{0,\pi\},\ \theta_R=0,\\
2^{-1}|z|^{-1/2}e^{\mathrm{Im}(z^{1/2})} + O\Big(|z|^{-1}e^{\mathrm{Im}(z^{1/2})R}\Big),\\
\hfill \theta_0=\theta_R=0.
\end{cases} \tag{3.57}
$$

Finally, combining (3.49) and (3.57) proves (3.53). □

Next, we recall an explicit formula for $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ in terms of the resolvent $(H_{\theta_0,\theta_R} - zI\big)^{-1}$ of H_{θ_0,θ_R} and the boundary traces $\gamma_{\theta_0',\theta_R'}$. We start with the Green's function for the operator H_{θ_0,θ_R} in (3.5),

$$
\begin{aligned}
&G_{\theta_0,\theta_R}(z,x,x') = (H_{\theta_0,\theta_R} - zI)^{-1}(x,x')\\
&\quad = \frac{1}{W(u_{+,\theta_R}(z,\cdot),u_{-,\theta_0}(z,\cdot))}\begin{cases} u_{-,\theta_0}(z,x')u_{+,\theta_R}(z,x), & 0\leqslant x'\leqslant x,\\ u_{-,\theta_0}(z,x)u_{+,\theta_R}(z,x'), & 0\leqslant x\leqslant x',\end{cases}\\
&\hspace{7cm} z\in\rho(H_{\theta_0,\theta_R}),\ x,x'\in[0,R].
\end{aligned} \tag{3.58}
$$

Here $u_{+,\theta_R}(z,\cdot), u_{-,\theta_0}(z,\cdot)$ is a basis for solutions of (3.15) as described in (3.17) and we denote by $I = I_{L^2((0,R);dx)}$ the identity operator in $L^2((0,R);dx)$. Thus, one obtains

$$
\begin{aligned}
&\big((H_{\theta_0,\theta_R} - zI)^{-1}g\big)(x) = \int_0^R dx'\, G_{\theta_0,\theta_R}(z,x,x')g(x'),\\
&\qquad g\in L^2((0,R);dx),\ z\in\rho(H_{\theta_0,\theta_R}),\ x\in(0,R).
\end{aligned} \tag{3.59}
$$

For future purposes we now introduce the following 2×2 matrix

$$
S_{\theta_0,\theta_R} = \begin{bmatrix} \sin(\theta_0) & 0\\ 0 & \sin(\theta_R)\end{bmatrix}. \tag{3.60}
$$

Theorem 3.6. *Assume that $\theta_0, \theta_R, \theta_0', \theta_R' \in S_{2\pi}$ and let H_{θ_0,θ_R} be defined as in* (3.5)*. Then*

$$\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) S_{\theta_0'-\theta_0,\theta_R'-\theta_R} = \gamma_{\theta_0',\theta_R'} \big[\gamma_{\overline{\theta_0'},\overline{\theta_R'}}((H_{\theta_0,\theta_R})^* - \overline{z}I)^{-1}\big]^*, \quad z \in \rho(H_{\theta_0,\theta_R}). \tag{3.61}$$

The fact that $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$ and $\Lambda_{\delta_0,\delta_R}^{\delta_0',\delta_R'}(z)$ satisfy a linear fractional transformation is recalled next:

Theorem 3.7. *Assume that $\theta_0, \theta_R, \theta_0', \theta_R', \delta_0, \delta_R, \delta_0', \delta_R' \in S_{2\pi}$, $\delta_0' - \delta_0 \neq 0 \,\mathrm{mod}(\pi)$, $\delta_R' - \delta_R \neq 0 \,\mathrm{mod}(\pi)$, and that $z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{\delta_0,\delta_R})$. Then, with S_{θ_0,θ_R} defined as in* (3.60),

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) &= \big(S_{\delta_0'-\delta_0,\delta_R'-\delta_R}\big)^{-1} \big[S_{\delta_0'-\theta_0',\delta_R'-\theta_R'} + S_{\theta_0'-\delta_0,\theta_R'-\delta_R} \Lambda_{\delta_0,\delta_R}^{\delta_0',\delta_R'}(z)\big] \\ &\quad \times \big[S_{\delta_0'-\theta_0,\delta_R'-\theta_R} + S_{\theta_0-\delta_0,\theta_R-\delta_R} \Lambda_{\delta_0,\delta_R}^{\delta_0',\delta_R'}(z)\big]^{-1} S_{\delta_0'-\delta_0,\delta_R'-\delta_R}. \end{aligned} \tag{3.62}$$

If in addition, $\theta_R' - \theta_R \neq 0 \,\mathrm{mod}(\pi)$, $\delta_0' - \delta_0 \neq 0 \,\mathrm{mod}(\pi)$, then

$$\begin{aligned} &\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) S_{\theta_0'-\theta_0,\theta_R'-\theta_R} \\ &\quad = \Big[S_{\delta_0'-\theta_0',\delta_R'-\theta_R'} + \big(S_{\delta_0'-\delta_0,\delta_R'-\delta_R}\big)^{-1} S_{\theta_0'-\delta_0,\theta_R'-\delta_R} \Lambda_{\delta_0,\delta_R}^{\delta_0',\delta_R'}(z) S_{\delta_0'-\delta_0,\delta_R'-\delta_R}\Big] \\ &\qquad \times \Big[\big(S_{\theta_0'-\theta_0,\theta_R'-\theta_R}\big)^{-1} S_{\delta_0'-\theta_0,\delta_R'-\theta_R} + \big(S_{\theta_0'-\theta_0,\theta_R'-\theta_R}\big)^{-1} \big(S_{\delta_0'-\delta_0,\delta_R'-\delta_R}\big)^{-1} \\ &\qquad\qquad \times S_{\theta_0-\delta_0,\theta_R-\delta_R} \Lambda_{\delta_0,\delta_R}^{\delta_0',\delta_R'}(z) S_{\delta_0'-\delta_0,\delta_R'-\delta_R}\Big]^{-1}. \end{aligned} \tag{3.63}$$

We denote by $\mathbb{C}_+$ the open complex upper half-plane and abbreviate $\mathrm{Im}(L) = (L - L^*)/(2i)$ for $L \in \mathbb{C}^{n\times n}$, $n \in \mathbb{N}$. In addition, $d\|\Sigma\|_{\mathbb{C}^{2\times 2}}$ will denote the total variation of the 2×2 matrix-valued measure $d\Sigma$ below in (3.65).

The matrix $M(\cdot)$ is called an $n \times n$ matrix-valued Herglotz function if it is analytic on $\mathbb{C}_+$ and $\mathrm{Im}(M(z)) \geq 0$ for all $z \in \mathbb{C}_+$. Now we are in position to recall the fundamental Herglotz property of the matrix $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot) S_{\theta_0'-\theta_0,\theta_R'-\theta_R}$ in the case where H_{θ_0,θ_R} is self-adjoint:

Theorem 3.8. *Let $\theta_0, \theta_R, \theta_0', \theta_R' \in [0, 2\pi)$, $\theta_0' - \theta_0 \neq 0 \,\mathrm{mod}(\pi)$, $\theta_R' - \theta_R \neq 0 \,\mathrm{mod}(\pi)$, $z \in \rho(H_{\theta_0,\theta_R})$, and H_{θ_0,θ_R} be defined as in* (3.5)*. In addition, suppose that V is real-valued* (*and hence H_{θ_0,θ_R} is self-adjoint*)*. Then $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot) S_{\theta_0'-\theta_0,\theta_R'-\theta_R}$ is a 2×2 matrix-valued Herglotz function admitting the representation*

$$\begin{aligned} \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) S_{\theta_0'-\theta_0,\theta_R'-\theta_R} = \Xi_{\theta_0,\theta_R}^{\theta_0',\theta_R'} + \int_{\mathbb{R}} d\Sigma_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\lambda) \bigg(\frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2}\bigg), \\ z \in \rho(H_{\theta_0,\theta_R}), \end{aligned} \tag{3.64}$$

$$\Xi_{\theta_0,\theta_R}^{\theta_0',\theta_R'} = \Big(\Xi_{\theta_0,\theta_R}^{\theta_0',\theta_R'}\Big)^* \in \mathbb{C}^{2\times 2}, \quad \int_{\mathbb{R}} \frac{d\big\|\Sigma_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\lambda)\big\|_{\mathbb{C}^{2\times 2}}}{1 + \lambda^2} < \infty, \tag{3.65}$$

where

$$\begin{aligned} \Sigma_{\theta_0,\theta_R}^{\theta_0',\theta_R'}((\lambda_1, \lambda_2]) = \frac{1}{\pi} \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \int_{\lambda_1+\delta}^{\lambda_2+\delta} d\lambda \, \mathrm{Im}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\lambda + i\varepsilon) S_{\theta_0'-\theta_0,\theta_R'-\theta_R}\Big), \\ \lambda_1, \lambda_2 \in \mathbb{R}, \ \lambda_1 < \lambda_2. \end{aligned} \tag{3.66}$$

In addition,

$$\operatorname{Im}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)S_{\theta_0'-\theta_0,\theta_R'-\theta_R}\Big) > 0, \quad z \in \mathbb{C}_+, \tag{3.67}$$

and

$$\operatorname{supp}\Big(d\Sigma_{\theta_0,\theta_R}^{\theta_0',\theta_R'}\Big) \subseteq \big(\sigma(H_{\theta_0,\theta_R}) \cup \sigma(H_{\theta_0',\theta_R'})\big), \tag{3.68}$$

in particular, $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot)S_{\theta_0'-\theta_0,\theta_R'-\theta_R}$ *is self-adjoint on* $\mathbb{R}\cap\rho(H_{\theta_0,\theta_R})\cap\rho(H_{\theta_0',\theta_R'})$.

We note that relation (3.68) is a consequence of (3.49) and of the fact that $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot)S_{\theta_0'-\theta_0,\theta_R'-\theta_R}$ is a meromorphic Herglotz matrix.

Remark 3.9. If $\theta_0'-\theta_0 = 0 \bmod(\pi)$ and $\theta_R'-\theta_R \neq 0 \bmod(\pi)$ (resp., $\theta_R'-\theta_R = 0 \bmod(\pi)$ and $\theta_0'-\theta_0 \neq 0 \bmod(\pi)$) then (3.30) shows that $\Lambda_{\theta_0,\theta_R}^{\theta_0,\theta_R'}(\cdot)S_{0,\theta_R'-\theta_R}$ (resp., $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R}(\cdot)S_{\theta_0'-\theta_0,0}$) is a diagonal matrix of the form

$$\Lambda_{\theta_0,\theta_R}^{\theta_0,\theta_R'}(\cdot)S_{0,\theta_R'-\theta_R} = \begin{pmatrix} 0 & 0 \\ 0 & m_{\theta_R}(\cdot)\end{pmatrix} \quad \left(\text{resp., } \Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R}(\cdot)S_{\theta_0'-\theta_0,0} = \begin{pmatrix} m_{\theta_0}(\cdot) & 0 \\ 0 & 0\end{pmatrix}\right), \tag{3.69}$$

with $m_{\theta_R}(\cdot)$ (resp., $m_{\theta_0}(\cdot)$) a scalar Herglotz function.

Finally, we briefly turn to a discussion of Krein-type resolvent formulas for the difference of resolvents of $H_{\theta_0',\theta_R'}$ and H_{θ_0,θ_R}:

Lemma 3.10. *Assume that* $\theta_0,\theta_R,\theta_0',\theta_R' \in S_{2\pi}$*, let* H_{θ_0,θ_R} *be defined as in* (3.5)*, and suppose that* $z\in\rho(H_{\theta_0,\theta_R})$*. Then, assuming* $f\in L^2((0,R);dx)$*, and writing*

$$\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R}-zI)^{-1}f = \begin{bmatrix} \big(\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R}-zI)^{-1}\big)_1 f \\ \big(\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R}-zI)^{-1}\big)_2 f\end{bmatrix} \in \mathbb{C}^2, \tag{3.70}$$

one has

$$\begin{aligned}\big(\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R}-zI)^{-1}\big)_1 f &= \frac{\sin(\theta_0'-\theta_0)}{W(u_{+,\theta_R}(z,\cdot),u_{-,\theta_0}(z,\cdot))}\big(\overline{u_{+,\theta_R}(z,\cdot)},f\big)_{L^2((0,R);dx)} \\ &\quad\times\begin{cases} -\frac{u_{-,\theta_0}(z,0)}{\sin(\theta_0)}, & \theta_0\in S_{2\pi}\backslash\{0,\pi\}, \\ \frac{u_{-,\theta_0}'(z,0)}{\cos(\theta_0)}, & \theta_0 \in S_{2\pi}\backslash\{\pi/2,3\pi/2\},\end{cases}\end{aligned} \tag{3.71}$$

$$\begin{aligned}\big(\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R}-zI)^{-1}\big)_2 f &= \frac{-\sin(\theta_R'-\theta_R)}{W(u_{+,\theta_R}(z,\cdot),u_{-,\theta_0}(z,\cdot))}\big(\overline{u_{-,\theta_0}(z,\cdot)},f\big)_{L^2((0,R);dx)} \\ &\quad\times\begin{cases} \frac{u_{+,\theta_R}(z,R)}{\sin(\theta_R)}, & \theta_R\in S_{2\pi}\backslash\{0,\pi\}, \\ \frac{u_{+,\theta_R}'(z,R)}{\cos(\theta_R)}, & \theta_R \in S_{2\pi}\backslash\{\pi/2,3\pi/2\},\end{cases}\end{aligned} \tag{3.72}$$

in addition,

$$\gamma_{\theta_0,\theta_R}(H_{\theta_0,\theta_R}-zI)^{-1} = 0 \ \text{ in } \mathcal{B}\big(L^2((0,R);dx),\mathbb{C}^2\big), \tag{3.73}$$

$$\big(\gamma_{\theta_0,\theta_R}(H_{\theta_0,\theta_R}-zI)^{-1}\big)_k = 0 \ \text{ in } \mathcal{B}\big(L^2((0,R);dx),\mathbb{C}\big), \ k=1,2. \tag{3.74}$$

Introducing the orthogonal projections in $\mathbb{C}^2$,

$$P_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0\end{bmatrix}, \quad P_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1\end{bmatrix}, \tag{3.75}$$

one obtains the following Krein-type resolvent formulas (cf. [1, Ch. 8], [3], [9]–[14], [23], [25], [26]–[28], [34], [43]–[45], [60], [63], [64], [67]):

Theorem 3.11. *Assume that $\theta_0, \theta_R, \theta_0', \theta_R' \in S_{2\pi}$, let H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ be defined as in* (3.5)*, and suppose that $z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{\theta_0',\theta_R'})$. Then, with $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot)$ introduced in* (3.23)*, and with S_{θ_0,θ_R} defined as in* (3.60)*,*

$$\begin{aligned}
&(H_{\theta_0',\theta_R'} - zI)^{-1} = (H_{\theta_0,\theta_R} - zI)^{-1} \\
&\quad - \big[\gamma_{\overline{\theta_0'},\overline{\theta_R'}}((H_{\theta_0,\theta_R})^* - \overline{z}I)^{-1}\big]^* S_{\theta_0'-\theta_0,\theta_R'-\theta_R}^{-1} \\
&\quad \times \Big[\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big]^{-1} \big[\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}\big], \quad \theta_0 \neq \theta_0', \ \theta_R \neq \theta_R'.
\end{aligned} \tag{3.76}$$

$$\begin{aligned}
&(H_{\theta_0,\theta_R'} - zI)^{-1} = (H_{\theta_0,\theta_R} - zI)^{-1} \\
&\quad - \big[\gamma_{\overline{\theta_0},\overline{\theta_R'}}((H_{\theta_0,\theta_R})^* - \overline{z}I)^{-1}\big]^* [\sin(\theta_R' - \theta_R)]^{-1} P_2 \\
&\quad \times \Big[\Lambda_{\theta_0,\theta_R}^{\theta_0,\theta_R'}(z)\Big]^{-1} P_2 \big[\gamma_{\theta_0,\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}\big], \quad \theta_R \neq \theta_R',
\end{aligned} \tag{3.77}$$

$$\begin{aligned}
&(H_{\theta_0',\theta_R} - zI)^{-1} = (H_{\theta_0,\theta_R} - zI)^{-1} \\
&\quad - \big[\gamma_{\overline{\theta_0'},\overline{\theta_R}}((H_{\theta_0,\theta_R})^* - \overline{z}I)^{-1}\big]^* [\sin(\theta_0' - \theta_0)]^{-1} P_1 \\
&\quad \times \Big[\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R}(z)\Big]^{-1} P_1 \big[\gamma_{\theta_0',\theta_R}(H_{\theta_0,\theta_R} - zI)^{-1}\big], \quad \theta_0 \neq \theta_0'.
\end{aligned} \tag{3.78}$$

4. Boundary Data Maps, Perturbation Determinants and Trace Formulas for Schrödinger Operators

In this section we present our second group of new results, the connection between boundary data maps, appropriate perturbation determinants, and trace formulas in the context of self-adjoint one-dimensional Schrödinger operators.

While Theorem 2.8 appears to be an interesting extension of the classical result, Theorem 2.1, it is in general, that is, in the context of non-self-adjoint operators, not a simple task to verify the hypotheses (2.30)–(2.32) as they involve square root domains. In particular, it appears to be unknown whether or not $\mathrm{dom}(H_{\theta_0,\theta_R})$ and $\mathrm{dom}((H_{\theta_0,\theta_R})^*)$ coincide and hence coincide with $\mathrm{dom}(Q_{H_{\theta_0,\theta_R}})$, the form domain of H_{θ_0,θ_R} (assuming H_{θ_0,θ_R} to be non-self-adjoint): This question amounts to solving "Kato's problem" in the special case of the non-self-adjoint Schrödinger operator H_{θ_0,θ_R} (cf., e.g., and [2], [6], [38], [52], [57], [58], and [59]), a topic we will return to elsewhere.

To be on safe ground, we now confine ourselves to the special case of self-adjoint operators H_{θ_0,θ_R} for the remainder of this section: Necessary and sufficient conditions for H_{θ_0,θ_R} to be self-adjoint are the conditions

$$V \in L^1((0,R);dx) \ \text{ is real-valued,} \tag{4.1}$$

and

$$\theta_0, \theta_R \in [0, 2\pi), \tag{4.2}$$

assumed from now on. Then the 2nd representation theorem for densely defined, semibounded, closed quadratic forms (cf. [39, Sect. 6.2.6]) yields that

$$\begin{aligned}
\mathrm{dom}((H_{\theta_0,\theta_R} - zI_{\mathcal{H}})^{1/2}) = \mathrm{dom}(|H_{\theta_0,\theta_R}|^{1/2}) = \mathrm{dom}(Q_{H_{\theta_0,\theta_R}}),& \\
\theta_0, \theta_R \in [0, 2\pi), \ z \in \mathbb{C}\backslash[e_{\theta_0,\theta_R}, \infty),&
\end{aligned} \tag{4.3}$$

where we abbreviated

$$e_{\theta_0,\theta_R} = \inf(\sigma(H_{\theta_0,\theta_R})), \quad \theta_0, \theta_R \in [0, 2\pi). \tag{4.4}$$

Here $(H_{\theta_0,\theta_R} - zI_{\mathcal{H}})^{1/2}$ is defined with the help of the spectral theorem and a choice of a branch cut along $[e_{\theta_0,\theta_R}, \infty)$. A comparison with (3.11)–(3.14), employing the fact that

$$\begin{aligned} &\operatorname{dom}((H_{\theta_0',\theta_R'} - zI_{\mathcal{H}})^{1/2}) = \operatorname{dom}(|H_{\theta_0',\theta_R'}|^{1/2}) = H^1((0,R)), \\ &\hspace{5cm} \theta_0', \theta_R' \in [0,2\pi)\backslash\{0,\pi\}, \ z \in \mathbb{C}\backslash[e_{\theta_0',\theta_R'}, \infty), \end{aligned} \tag{4.5}$$

$$\begin{aligned} &\operatorname{dom}((H_{\theta_0,\theta_R} - zI_{\mathcal{H}})^{1/2}) = \operatorname{dom}(|H_{\theta_0,\theta_R}|^{1/2}) \subseteq H^1((0,R)), \\ &\hspace{6cm} \theta_0, \theta_R \in [0,2\pi), \ z \in \mathbb{C}\backslash[e_{\theta_0,\theta_R}, \infty), \end{aligned} \tag{4.6}$$

then shows that

$$\begin{aligned} &\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}} \\ &\quad = \big[(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1/2}\big] \\ &\qquad \times \big[(H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2}(H_{\theta_0,\theta_R} - \overline{z}I)^{-1/2}\big]^* \in \mathcal{B}\big(L^2((0,R);dx)\big), \\ &\qquad\quad \theta_0', \theta_R' \in [0,2\pi)\backslash\{0,\pi\}, \ \theta_0, \theta_R \in [0,2\pi), \ z \in \mathbb{C}\backslash[e_0, \infty), \end{aligned} \tag{4.7}$$

where we introduced the abbreviation

$$e_0 = \inf\big(\sigma(H_{\theta_0,\theta_R}) \cup \sigma(H_{\theta_0',\theta_R'})\big) = \min(e_{\theta_0,\theta_R}, e_{\theta_0',\theta_R'}). \tag{4.8}$$

Moreover, applying Theorem 3.11 one concludes that actually,

$$\begin{aligned} &\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}} - I \\ &\quad = -\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}\big[(H_{\theta_0',\theta_R'} - zI)^{-1} - (H_{\theta_0,\theta_R} - zI)^{-1}\big](H_{\theta_0',\theta_R'} - zI)^{1/2}} \\ &\qquad \text{is a finite-rank (and hence a trace class operator) on } L^2((0,R);dx), \\ &\qquad\qquad \theta_0', \theta_R' \in [0,2\pi)\backslash\{0,\pi\}, \ \theta_0, \theta_R \in [0,2\pi), \ z \in \mathbb{C}\backslash[e_0, \infty). \end{aligned} \tag{4.9}$$

To see the finite-rank property one can argue as follows: By (3.70)–(3.72), the $\mathbb{C}^2$-vector $\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}f$, $f \in L^2\big((0,R);dx\big)$, is of the type

$$\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}f = \begin{bmatrix} C_1\big(\overline{u_{+,\theta_R}(z,\cdot)}, f\big)_{L^2((0,R);dx)} \\ C_2\big(\overline{u_{-,\theta_0}(z,\cdot)}, f\big)_{L^2((0,R);dx)} \end{bmatrix}, \tag{4.10}$$

for some $C_j = C_j(z, \theta_0', \theta_R', \theta_0, \theta_R)$, $j = 1, 2$, and hence, since obviously $u_{+,\theta_R}(z,\cdot)$ and $u_{-,\theta_0}(z,\cdot)$ belong to $H^1((0,R))$,

$$\begin{aligned} &\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}g \\ &\quad = \begin{bmatrix} C_1\big(\overline{u_{+,\theta_R}(z,\cdot)}, (H_{\theta_0',\theta_R'} - zI)^{1/2}g\big)_{L^2((0,R);dx)} \\ C_2\big(\overline{u_{-,\theta_0}(z,\cdot)}, (H_{\theta_0',\theta_R'} - zI)^{1/2}g\big)_{L^2((0,R);dx)} \end{bmatrix} \\ &\quad = \begin{bmatrix} C_1\big([(H_{\theta_0',\theta_R'} - zI)^{1/2}]^*\overline{u_{+,\theta_R}(z,\cdot)}, g\big)_{L^2((0,R);dx)} \\ C_2\big([(H_{\theta_0',\theta_R'} - zI)^{1/2}]^*\overline{u_{-,\theta_0}(z,\cdot)}, g\big)_{L^2((0,R);dx)} \end{bmatrix}, \quad g \in H^1((0,R)), \end{aligned} \tag{4.11}$$

extends by continuity to all $g \in L^2\big((0,R);dx\big)$. Similarly, using [14, eq. (3.54)], one infers for any $[a_0 \ \ a_R]^\top \in \mathbb{C}^2$ that

$$\begin{aligned} &\big[\gamma_{\theta_0',\theta_R'}((H_{\theta_0,\theta_R})^* - \overline{z}I)^{-1}\big]^*[a_0 \ \ a_R]^\top \\ &\quad = D_1 a_0 u_{+,\theta_R}(z,\cdot) + D_2 a_R u_{-,\theta_0}(z,\cdot) \in H^1((0,R)), \end{aligned} \tag{4.12}$$

for some $D_j = D_j(z, \theta_0', \theta_R', \theta_0, \theta_R)$, $j = 1, 2$. Consequently,

$$(H_{\theta_0',\theta_R'} - zI)^{1/2}\big[\gamma_{\theta_0',\theta_R'}((H_{\theta_0,\theta_R})^* - \overline{z}I)^{-1}\big]^*[a_0 \;\; a_R]^\top \in L^2\big((0,R); dx\big) \tag{4.13}$$

is well-defined for all $[a_0 \;\; a_R]^\top \in \mathbb{C}^2$. Thus, combining (4.11) (for arbitrary $g \in L^2\big((0,R); dx\big)$) and (4.13) (for arbitrary $[a_0 \;\; a_R]^\top \in \mathbb{C}^2$) with the finite-rank property of the second terms on the right-hand sides in (3.76)–(3.78) yields the asserted finite-rank property in (4.9).

Thus, the Fredholm determinant, more precisely, the symmetrized perturbation determinant,

$$\begin{aligned}
&\det_{L^2((0,R);dx)}\Big(\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}}\Big), \\
&\qquad\qquad \theta_0, \theta_R \in [0, 2\pi), \; \theta_0', \theta_R' \in (0, 2\pi)\backslash\{\pi\}, \; z \in \mathbb{C}\backslash[e_0, \infty),
\end{aligned} \tag{4.14}$$

is well-defined, and an application of Theorem 2.8 to $H_{\theta_0',\theta_R'}$ and H_{θ_0,θ_R} yields

$$\begin{aligned}
&\operatorname{tr}_{L^2((0,R);dx)}\big((H_{\theta_0',\theta_R'} - zI)^{-1} - (H_{\theta_0,\theta_R} - zI)^{-1}\big) \\
&\quad = -\frac{d}{dz}\ln\Big(\det_{L^2((0,R);dx)}\Big(\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}}\Big)\Big), \\
&\qquad\qquad \theta_0, \theta_R \in [0, 2\pi), \; \theta_0', \theta_R' \in (0, 2\pi)\backslash\{\pi\}, \; z \in \mathbb{C}\backslash[e_0, \infty),
\end{aligned} \tag{4.15}$$

whenever $\det_{L^2((0,R);dx)}\Big(\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}}\Big) \neq 0$.

Next, we show that the symmetrized (Fredholm) perturbation determinant (4.14) can essentially be reduced to the 2×2 determinant of the boundary data map $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)$:

Theorem 4.1. *Assume that* $\theta_0, \theta_R \in [0, 2\pi)$, $\theta_0', \theta_R' \in (0, 2\pi)\backslash\{\pi\}$, *and suppose that* V *satisfies* (4.1). *Let* H_{θ_0,θ_R} *and* $H_{\theta_0',\theta_R'}$ *be defined as in* (3.5). *Then,*

$$\begin{aligned}
&\det_{L^2((0,R);dx)}\Big(\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}}\Big) \\
&\quad = \frac{\sin(\theta_0)\sin(\theta_R)}{\sin(\theta_0')\sin(\theta_R')}\det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big), \quad z \in \mathbb{C}\backslash[e_0, \infty).
\end{aligned} \tag{4.16}$$

Proof. Let $z \in \mathbb{C}\backslash[e_0, \infty)$. By (3.8) and (3.9) it suffices to consider $\theta_0, \theta_R \in [0, \pi)$, $\theta_0', \theta_R' \in (0, \pi)$. Moreover, we will assume that $\theta_0 \neq 0$ and $\theta_R \neq 0$. The cases where $\theta_0 = 0$ and/or $\theta_R = 0$ follow along the same lines.

In addition, simplifying the proof a bit, we will choose $z < 0$, $|z|$ sufficiently large, and introduce the following convenient abbreviations:

$$\begin{aligned}
&H = H_{\theta_0,\theta_R}, \quad H' = H_{\theta_0',\theta_R'}, \quad \gamma = \gamma_{\theta_0,\theta_R}, \quad \gamma' = \gamma_{\theta_0',\theta_R'}, \\
&\Lambda(z) = \Lambda_{\theta_0',\theta_R'}^{\theta_0,\theta_R}(z), \quad S = S_{\theta_0-\theta_0',\theta_R-\theta_R'} = \begin{pmatrix} \sin(\theta_0 - \theta_0') & 0 \\ 0 & \sin(\theta_R - \theta_R') \end{pmatrix}, \\
&\breve{u}_+(z, \cdot) = u_{+,\theta_R'}(z, \cdot), \quad \breve{u}_-(z, \cdot) = u_{-,\theta_0'}(z, \cdot), \\
&\breve{W}(z) = W(\breve{u}_+(z, \cdot), \breve{u}_-(z, \cdot)) = W(u_{+,\theta_R'}(z, \cdot), u_{-,\theta_0'}(z, \cdot)), \\
&B(z) = (H' - zI)^{1/2}\big[\gamma(H' - zI)^{-1}\big]^* \in \mathcal{B}\big(\mathbb{C}^2, L^2((0,R); dx)\big).
\end{aligned} \tag{4.17}$$

That $B(z) \in \mathcal{B}\big(\mathbb{C}^2, L^2((0,R); dx)\big)$ follows as in (4.12), (4.13). In addition, we recall that

$$\big[\gamma(H' - zI)^{-1}\big]^*(a_0 \; a_R)^\top = \frac{\sin(\theta_0)}{\breve{W}(z)}[\breve{u}_-'(z, 0) + \cot(\theta_0)\breve{u}_-(z, 0)]a_0\breve{u}_+(z, \cdot)$$

$$- \frac{\sin(\theta_R)}{\breve{W}(z)}[\breve{u}_+'(z,R) - \cot(\theta_R)\breve{u}_+(z,R)]a_R\breve{u}_-(z,\cdot), \quad (a_0\ a_R)^\top \in \mathbb{C}^2 \tag{4.18}$$

(cf. [14, eq. (3.54)]). Thus,

$$\begin{aligned} B(z)(a_0\ a_R)^\top &= \frac{\sin(\theta_0)}{\breve{W}(z)}[\breve{u}_-'(z,0) + \cot(\theta_0)\breve{u}_-(z,0)]a_0(H'-zI)^{1/2}\breve{u}_+(z,\cdot) \\ &\quad - \frac{\sin(\theta_R)}{\breve{W}(z)}[\breve{u}_+'(z,R) - \cot(\theta_R)\breve{u}_+(z,R)]a_R(H'-zI)^{1/2}\breve{u}_-(z,\cdot), \\ &\hspace{8cm} (a_0\ a_R)^\top \in \mathbb{C}^2, \end{aligned} \tag{4.19}$$

and hence $B(z)^* \in \mathcal{B}\big(L^2((0,R);dx), \mathbb{C}^2\big)$ is given by

$$\begin{aligned} &B(z)^* f \\ &\quad = \begin{pmatrix} \frac{\sin(\theta_0)}{\breve{W}(z)}[\breve{u}_-'(z,0) + \cot(\theta_0)\breve{u}_-(z,0)]((H'-zI)^{1/2}\breve{u}_+(z,\cdot), f)_{L^2((0,R);dx)} \\ -\frac{\sin(\theta_R)}{\breve{W}(z)}[\breve{u}_+'(z,R) - \cot(\theta_R)\breve{u}_+(z,R)]((H'-zI)^{1/2}\breve{u}_-(z,\cdot), f)_{L^2((0,R);dx)} \end{pmatrix}, \\ &\hspace{8cm} f \in L^2((0,R);dx). \end{aligned} \tag{4.20}$$

Using the following version of the Krein-type resolvent formula (3.76)

$$(H-zI)^{-1} = (H'-zI)^{-1} - \big[\gamma(H'-zI)^{-1}\big]^* S^{-1}\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}\big[\gamma(H'-zI)^{-1}\big], \tag{4.21}$$

one obtains

$$\begin{aligned} &\overline{(H'-zI)^{1/2}(H-zI)^{-1}(H'-zI)^{1/2}} \\ &\quad = I - \overline{(H'-zI)^{1/2}\big[(H'-zI)^{-1} - (H-zI)^{-1}\big](H'-zI)^{1/2}} \\ &\quad = I - B(z)S^{-1}\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}B(z)^*, \end{aligned} \tag{4.22}$$

and thus,

$$\begin{aligned} &\det{}_{L^2((0,R);dx)}\Big(\overline{(H'-zI)^{1/2}(H-zI)^{-1}(H'-zI)^{1/2}}\Big) \\ &\quad = \det{}_{L^2((0,R);dx)}\Big(I - B(z)S^{-1}\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}B(z)^*\Big) \\ &\quad = \det{}_{\mathbb{C}^2}\Big(I_2 - S^{-1}\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}B(z)^*B(z)\Big), \end{aligned} \tag{4.23}$$

using cyclicity for determinants .

Next we turn to the computation of the 2×2 matrix $B(z)^*B(z)$: By equations (4.19) and (4.20) one infers

$$B(z)^*B(z) = \big(C_{j,k}(z)\big)_{j,k=1,2}, \tag{4.24}$$

$$\begin{aligned} C_{1,1}(z) &= \frac{\sin^2(\theta_0)}{\breve{W}(z)^2}[\breve{u}_-'(z,0) + \cot(\theta_0)\breve{u}_-(z,0)]^2 \\ &\quad \times ((H'-zI)^{1/2}\breve{u}_+(z,\cdot), (H'-zI)^{1/2}\breve{u}_+(z,\cdot))_{L^2((0,R);dx)}, \end{aligned} \tag{4.25}$$

$$\begin{aligned} C_{1,2}(z) &= -\frac{\sin(\theta_0)\sin(\theta_R)}{\breve{W}(z)^2} \\ &\quad \times [\breve{u}_-'(z,0) + \cot(\theta_0)\breve{u}_-(z,0)][\breve{u}_+'(z,R) - \cot(\theta_R)\breve{u}_+(z,R)] \\ &\quad \times ((H'-zI)^{1/2}\breve{u}_+(z,\cdot), (H'-zI)^{1/2}\breve{u}_-(z,\cdot))_{L^2((0,R);dx)}, \end{aligned} \tag{4.26}$$

$$\begin{aligned}
C_{2,1}(z) = &-\frac{\sin(\theta_0)\sin(\theta_R)}{\check W(z)^2} \\
&\times [\check u_-'(z,0)+\cot(\theta_0)\check u_-(z,0)][\check u_+'(z,R)-\cot(\theta_R)\check u_+(z,R)] \\
&\times ((H'-zI)^{1/2}\check u_-(z,\cdot),(H'-zI)^{1/2}\check u_+(z,\cdot))_{L^2((0,R);dx)}, \qquad (4.27)\\
C_{2,2}(z) = &\frac{\sin^2(\theta_R)}{\check W(z)^2}[\check u_+'(z,R)-\cot(\theta_R)\check u_+(z,R)]^2 \\
&\times ((H'-zI)^{1/2}\check u_-(z,\cdot),(H'-zI)^{1/2}\check u_-(z,\cdot))_{L^2((0,R);dx)}. \qquad (4.28)
\end{aligned}$$

A straightforward, although rather tedious computation then yields the following simplification of $C_{j,k}(z)$, $j,k=1,2$, and hence of $B(z)^*B(z)$:

$$\begin{aligned}
C_{1,1}(z) &= -\frac{\sin^2(\theta_0-\theta_0')}{\sin^2(\theta_0')}\frac{1}{\check u_+'(z,0)+\cot(\theta_0')}, &(4.29)\\
C_{1,2}(z) &= \frac{\sin(\theta_0-\theta_0')\sin(\theta_R-\theta_R')}{\sin(\theta_0')\sin(\theta_R')}\frac{\check u_-(z,0)}{\check u_-'(z,R)-\cot(\theta_R')} &(4.30)\\
&= -\frac{\sin(\theta_0-\theta_0')\sin(\theta_R-\theta_R')}{\sin(\theta_0')\sin(\theta_R')}\frac{\check u_+(z,R)}{\check u_+'(z,0)+\cot(\theta_0')} &(4.31)\\
&= C_{2,1}(z), &(4.32)\\
C_{2,2}(z) &= \frac{\sin^2(\theta_R-\theta_R')}{\sin^2(\theta_R')}\frac{1}{\check u_-'(z,R)-\cot(\theta_R')}. &(4.33)
\end{aligned}$$

To arrrive at (4.29)–(4.33) one repeatedly uses the identity

$$\cot(x)-\cot(y) = \frac{\sin(y-x)}{\sin(y)\sin(x)}, \tag{4.34}$$

the following expressions for the Wronskian $\check W$,

$$\begin{aligned}
\check W(z) &= \check u_+(z,R)[\check u_-'(z,R)-\cot(\theta_R')] \\
&= -\check u_-(z,0)[\check u_+'(z,0)+\cot(\theta_0')],
\end{aligned} \tag{4.35}$$

and

$$\begin{aligned}
&((H'-zI)^{1/2}\check u_+(z,\cdot),(H'-zI)^{1/2}\check u_+(z,\cdot))_{L^2((0,R);dx)} \\
&\quad = -[\check u_+'(z,0)+\cot(\theta_0')], &(4.36)\\
&((H'-zI)^{1/2}\check u_+(z,\cdot),(H'-zI)^{1/2}\check u_-(z,\cdot))_{L^2((0,R);dx)} \\
&\quad = -\check u_-(z,0)[\check u_+'(z,0)+\cot(\theta_0')] = \check u_+(z,R)[\check u_-'(z,R)-\cot(\theta_R')], &(4.37)\\
&\quad = ((H'-zI)^{1/2}\check u_-(z,\cdot),(H'-zI)^{1/2}\check u_+(z,\cdot))_{L^2((0,R);dx)}, \\
&((H'-zI)^{1/2}\check u_-(z,\cdot),(H'-zI)^{1/2}\check u_-(z,\cdot))_{L^2((0,R);dx)} \\
&\quad = [\check u_-'(z,R)-\cot(\theta_R')]. &(4.38)
\end{aligned}$$

Relations (4.36)–(4.38) are a consequence of one integration by parts in (3.11).

Finally, we compute $\Lambda(z)S$, starting with (3.29) and (4.17):

$$\begin{aligned}
\Lambda(z)S &= \big(K_{j,k}(z)\big)_{j,k=1,2}, &(4.39)\\
K_{1,1}(z) &= \frac{\sin(\theta_0-\theta_0')\sin(\theta_0)}{\sin(\theta_0')}\frac{\check u_+'(z,0)+\cot(\theta_0)}{\check u_+'(z,0)+\cot(\theta_0')}
\end{aligned}$$

$$= C_{1,1}(z) + \frac{\sin(\theta_0 - \theta_0')\sin(\theta_0)}{\sin(\theta_0')}, \tag{4.40}$$

$$\begin{aligned}
K_{1,2}(z) &= -\frac{\sin(\theta_R - \theta_R')\sin(\theta_0)}{\sin(\theta_R')} \frac{\breve u_-(z,0) + \cot(\theta_0)\breve u_-(z,0)}{\breve u_-'(z,R) - \cot(\theta_R')} \\
&= \frac{\sin(\theta_0 - \theta_0')\sin(\theta_R - \theta_R')}{\sin(\theta_0')\sin(\theta_R')} \frac{\breve u_-(z,0)}{\breve u_-'(z,R) - \cot(\theta_R')} \\
&= C_{1,2}(z) = C_{2,1}(z) \qquad (4.41) \\
&= -\frac{\sin(\theta_0 - \theta_0')\sin(\theta_R - \theta_R')}{\sin(\theta_0')\sin(\theta_R')} \frac{\breve u_+(z,R)}{\breve u_+'(z,0) + \cot(\theta_0')} \\
&= K_{2,1}(z), \qquad (4.42) \\
K_{2,2}(z) &= \frac{\sin(\theta_R - \theta_R')\sin(\theta_R)}{\sin(\theta_R')} \frac{\breve u_-'(z,R) - \cot(\theta_R)}{\breve u_-'(z,R) + \cot(\theta_R')} \\
&= C_{2,2}(z) + \frac{\sin(\theta_R - \theta_R')\sin(\theta_R)}{\sin(\theta_R')}. \qquad (4.43)
\end{aligned}$$

In particular,

$$\Lambda(z)S = B(z)^*B(z) + \begin{pmatrix} \frac{\sin(\theta_0-\theta_0')\sin(\theta_0)}{\sin(\theta_0')} & 0 \\ 0 & \frac{\sin(\theta_R-\theta_R')\sin(\theta_R)}{\sin(\theta_R')} \end{pmatrix}. \tag{4.44}$$

An insertion of (4.44) into (4.23) finally yields

$$\begin{aligned}
&{\det}_{L^2((0,R);dx)}\Big(\overline{(H'-zI)^{1/2}(H-zI)^{-1}(H'-zI)^{1/2}}\Big) \\
&\quad = {\det}_{\mathbb{C}^2}\Big(I_2 - S^{-1}\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}B(z)^*B(z)\Big), \\
&\quad = {\det}_{\mathbb{C}^2}\left(I_2 - [\Lambda(z)S]^{-1}\left[\Lambda(z)S - \begin{pmatrix} \frac{\sin(\theta_0-\theta_0')\sin(\theta_0)}{\sin(\theta_0')} & 0 \\ 0 & \frac{\sin(\theta_R-\theta_R')\sin(\theta_R)}{\sin(\theta_R')} \end{pmatrix}\right]\right) \\
&\quad = {\det}_{\mathbb{C}^2}\left([\Lambda(z)S]^{-1}\begin{pmatrix} \frac{\sin(\theta_0-\theta_0')\sin(\theta_0)}{\sin(\theta_0')} & 0 \\ 0 & \frac{\sin(\theta_R-\theta_R')\sin(\theta_R)}{\sin(\theta_R')} \end{pmatrix}\right) \\
&\quad = {\det}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big){\det}_{\mathbb{C}^2}\big(S^{-1}\big)\frac{\sin(\theta_0-\theta_0')\sin(\theta_R-\theta_R')\sin(\theta_0)\sin(\theta_R)}{\sin(\theta_0')\sin(\theta_R')} \\
&\quad = \frac{\sin(\theta_0)\sin(\theta_R)}{\sin(\theta_0')\sin(\theta_R')}{\det}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big). \qquad (4.45)
\end{aligned}$$

□

Since the Fredholm determinant on the left-hand side of (4.16) vanishes for $\theta_0 = 0$ and/or $\theta_R = 0$, we now briefly consider the nullspace of the operators involved:.

Lemma 4.2. *Assume that $\theta_0, \theta_R \in [0, 2\pi)$, $\theta_0', \theta_R' \in (0, 2\pi)\backslash\{\pi\}$, $z \in \mathbb{C}\backslash[e_0,\infty)$, and suppose that V satisfies (4.1). Let H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ be defined as in (3.5). Then recalling the factorization,*

$$\begin{aligned}
&\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}} \qquad (4.46) \\
&\quad = (H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1/2}\big[(H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2}(H_{\theta_0,\theta_R} - \overline{z}I)^{-1/2}\big]^*
\end{aligned}$$

one obtains

$$\begin{aligned}
&\ker\big(\big[(H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}(H_{\theta_0,\theta_R}-\overline{z}I)^{-1/2}\big]^*\big)\\
&\quad=\big\{f\in L^2((0,R);dx)\,\big|\,f=(H_{\theta_0',\theta_R'}-zI)^{1/2}\psi(z,\cdot);\\
&\qquad\psi(z,\cdot),\psi'(z,\cdot)\in AC([0,R]);\ -\psi''(z,\cdot)+(V(\cdot)-z)\psi(z,\cdot)=0;\\
&\qquad\psi'(z,R)-\cot(\theta_R')\psi(z,R)=0\ \textit{if}\ \theta_0=0,\ \theta_R\neq0;\\
&\qquad\psi'(z,0)+\cot(\theta_0')\psi(z,0)=0\ \textit{if}\ \theta_0\neq0,\ \theta_R=0\\
&\qquad\textit{no boundary conditions on}\ \psi(z,\cdot)\ \textit{if}\ \theta_0=\theta_R=0\big\},
\end{aligned} \tag{4.47}$$

in particular,

$$\begin{aligned}
&\dim\big(\ker\big(\big[(H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}(H_{\theta_0,\theta_R}-\overline{z}I)^{-1/2}\big]^*\big)\big)\\
&\quad=\begin{cases}2, & \theta_0=\theta_R=0,\\ 1, & \theta_0=0,\ \theta_R\neq0\ \ \textit{or}\ \ \theta_0\neq0,\ \theta_R=0.\end{cases}
\end{aligned} \tag{4.48}$$

Proof. Let $z\in\mathbb{C}\backslash[e_0,\infty)$. To determine the precise characterization of the nullspace in (4.47) one can argue as follows: Suppose first that $\theta_0=\theta_R=0$ and that

$$\begin{aligned}
&f\perp\operatorname{ran}\big((H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}(H_{0,0}-\overline{z}I)^{-1/2}\big),\\
&g\in\operatorname{ran}\big((H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}(H_{0,0}-\overline{z}I)^{-1/2}\big),
\end{aligned} \tag{4.49}$$

implying

$$g=(H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}h\ \text{ for some }\ h\in H_0^1((0,R)), \tag{4.50}$$

and hence $h(0)=h(R)=0$. Thus, introducing $\psi(z,\cdot)=(H_{\theta_0',\theta_R'}-zI)^{-1/2}f$, one obtains using (3.11) again,

$$\begin{aligned}
0&=(g,f)_{L^2((0,R);dx)}\\
&=\big((H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}h,(H_{\theta_0',\theta_R'}-zI)^{1/2}(H_{\theta_0',\theta_R'}-zI)^{-1/2}f\big)_{L^2((0,R);dx)}\\
&=\big((H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}h,(H_{\theta_0',\theta_R'}-zI)^{1/2}\psi(z)\big)_{L^2((0,R);dx)}\\
&=\int_0^R dx\,[\overline{h'(x)}\psi'(z,x)+(V(x)-z)\overline{h(x)}\psi(z,x)]\\
&\quad-\cot(\theta_0')\overline{h(0)}\psi(z,0)-\cot(\theta_R')\overline{h(R)}\psi(z,R)\\
&=\overline{h(x)}\psi'(z,x)\big|_0^R+\int_0^R dx\,\overline{h(x)}[\psi''(z,x)+(V(x)-z)\psi(z,x)]\\
&=\int_0^R dx\,\overline{h(x)}[\psi''(z,x)+(V(x)-z)\psi(z,x)],\quad h\in H_0^1((0,R)).
\end{aligned} \tag{4.51}$$

Hence one concludes that

$$\psi(z,\cdot),\ \psi'(z,\cdot)\in AC([0,R]), \tag{4.52}$$

and that

$$\psi''(z,\cdot)+(V(\cdot)-z)\psi(z,\cdot)=0\ \text{ in the sense of distributions.} \tag{4.53}$$

As $g\in\operatorname{ran}\big((H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}(H_{0,0}-\overline{z}I)^{-1/2}\big)$ was chosen arbitrarily, one concludes that any element f in $\ker\big(\big[(H_{\theta_0',\theta_R'}-\overline{z}I)^{1/2}(H_{0,0}-\overline{z}I)^{-1/2}\big]^*\big)$ is of the form

$$f=(H_{\theta_0',\theta_R'}-zI)^{1/2}\psi(z,\cdot). \tag{4.54}$$

The fact that $\psi(z,\cdot)$ satisfies no boundary conditions then shows that the dimension of the nullspace in (4.47) is precisely two if $\theta_0 = \theta_R = 0$.

Next we consider the case $\theta_0 = 0$, $\theta_R \neq 0$ (the case $\theta_0 \neq 0$, $\theta_R = 0$ being completely analogous): Again we assume

$$\begin{aligned} &f \perp \operatorname{ran}\big((H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2}(H_{0,\theta_R} - \overline{z}I)^{-1/2}\big), \\ &g \in \operatorname{ran}\big((H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2}(H_{0,\theta_R} - \overline{z}I)^{-1/2}\big), \end{aligned} \tag{4.55}$$

implying

$$g = (H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2} h \text{ for some } h \in H^1((0,R)) \text{ with } h(0) = 0. \tag{4.56}$$

Introducing once more $\psi(z,\cdot) = (H_{\theta_0',\theta_R'} - zI)^{-1/2} f$, one obtains again via (3.11) that

$$\begin{aligned} 0 &= (g,f)_{L^2((0,R);dx)} \\ &= \big((H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2} h, (H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0',\theta_R'} - zI)^{-1/2} f\big)_{L^2((0,R);dx)} \\ &= \big((H_{\theta_0',\theta_R'} - \overline{z}I)^{1/2} h, (H_{\theta_0',\theta_R'} - zI)^{1/2}\psi(z)\big)_{L^2((0,R);dx)} \\ &= \int_0^R dx\, [\overline{h'(x)}\psi'(z,x) + (V(x)-z)\overline{h(x)}\psi(z,x)] \\ &\quad - \cot(\theta_0')\overline{h(0)}\psi(z,0) - \cot(\theta_R')\overline{h(R)}\psi(z,R) \\ &= \overline{h(x)}\psi'(z,x)\big|_0^R + \int_0^R dx\, \overline{h(x)}[\psi''(z,x) + (V(x)-z)\psi(z,x)] \\ &\quad - \cot(\theta_R')\overline{h(R)}\psi(z,R) \\ &= \overline{h(R)}[\psi'(z,R) - \cot(\theta_R')\psi(z,R)] \\ &\quad + \int_0^R dx\, \overline{h(x)}[\psi''(z,x) + (V(x)-z)\psi(z,x)], \quad h \in H^1((0,R)),\ h(0) = 0. \end{aligned} \tag{4.57}$$

Choosing temporarily $h \in H_0^1((0,R))$, one obtains

$$\int_0^R dx\, \overline{h(x)}[\psi''(z,x) + (V(x)-z)\psi(z,x)], \quad h \in H_0^1((0,R)), \tag{4.58}$$

and hence again concludes that

$$\psi(z,\cdot),\ \psi'(z,\cdot) \in AC([0,R]), \tag{4.59}$$

and that

$$\psi''(z,\cdot) + (V(\cdot) - z)\psi(z,\cdot) = 0 \text{ in the sense of distributions.} \tag{4.60}$$

Taking into account (4.60) in (4.57) then yields

$$0 = \overline{h(R)}[\psi'(z,R) - \cot(\theta_R')\psi(z,R)], \quad h \in H^1((0,R)),\ h(0) = 0, \tag{4.61}$$

implying

$$[\psi'(z,R) - \cot(\theta_R')\psi(z,R)] = 0. \tag{4.62}$$

As before, this proves (4.47) in the case $\theta_0 = 0$, $\theta_R \neq 0$. The boundary condition (4.62) then yields that the nullspace (4.47) is one-dimensional in this case. $\square$

Remark 4.3. We emphasize the interesting fact that relation (4.16) represents yet another reduction of an infinite-dimensional Fredholm determinant (more precisely, a symmetrized perturbation determinant) to a finite-dimensional determinant. This is analogous to the following well-known situations:
(i) The Jost–Pais formula [37] in the context of half-line Schrödinger operators (relating the perturbation determinant of the corresponding Birman–Schwinger kernel with the Jost function and hence a Wronski determinant).
(ii) Schrödinger operators on the real line [61] (relating the perturbation determinant of the corresponding Birman–Schwinger kernel with the transmission coefficient and hence again a Wronski determinant).
(iii) One-dimensional periodic Schrödinger operators [54] (relating the Floquet discriminant with an appropriate Fredholm determinant).
These cases, and much more general situations in connection with semi-separable integral kernels (which typically apply to one-dimensional differential and difference operators with matrix-valued coefficients) were studied in great deal in [24] (see also [30] and the multi-dimensional discussion in [29]).

We conclude this section by pointing out that determinants (especially, ζ-function regularized determinants) for various elliptic boundary value problems on compact intervals (including cases with regular singular coefficients) have received considerable attention and we refer, for instance, to Burghelea, Friedlander, and Kappeler [13], Dreyfus and Dym [19], Forman [22], Kirsten, Loya, and Park [40], Kirsten and McKane [41], Lesch [48], Lesch and Tolksdorf [49], Lesch and Vertman [50], and Levit and Smilansky [51] in this context.

5. Trace Formulas and the Spectral Shift Function

In this section we derive the trace formula for the resolvent difference of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ in terms of the spectral shift function $\xi(\cdot; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$ and establish the connection between $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot)$ and $\xi(\cdot; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$.

To prepare the ground for the basic trace formula we now state the following fact (which does not require H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ to be self-adjoint):

Lemma 5.1. *Assume that $\theta_0, \theta_R, \theta_0', \theta_R' \in S_{2\pi}$, and let H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ be defined as in* (3.5). *Then, with $\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot) S_{\theta_0'-\theta_0,\theta_R'-\theta_R}$ given by* (3.61),

$$\gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}\big[\gamma_{\overline{\theta_0'},\overline{\theta_R'}}(H_{\theta_0,\theta_R}^* - \overline{z}I)^{-1}\big]^* = \frac{d}{dz}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z) S_{\theta_0'-\theta_0,\theta_R'-\theta_R}\Big),\quad z \in \rho(H_{\theta_0,\theta_R}). \tag{5.1}$$

Proof. Employing the resolvent equation for H_{θ_0,θ_R}^*, one verifies that

$$\begin{aligned}\frac{d}{dz}\gamma_{\theta_0',\theta_R'}\big[\gamma_{\overline{\theta_0'},\overline{\theta_R'}}(H_{\theta_0,\theta_R}^* - \overline{z}I)^{-1}\big]^* &= \gamma_{\theta_0',\theta_R'}\big[\gamma_{\overline{\theta_0'},\overline{\theta_R'}}(H_{\theta_0,\theta_R}^* - \overline{z}I)^{-2}\big]^* \\ &= \gamma_{\theta_0',\theta_R'}(H_{\theta_0,\theta_R} - zI)^{-1}\big[\gamma_{\overline{\theta_0'},\overline{\theta_R'}}(H_{\theta_0,\theta_R}^* - \overline{z}I)^{-1}\big]^*.\end{aligned} \tag{5.2}$$

Together with (3.61) this proves (5.1). ∎

Combining Theorems 3.11 and 2.8 with Lemma 5.1 then yields the following result:

Theorem 5.2. *Assume that* $\theta_0, \theta_R, \theta_0', \theta_R' \in [0, 2\pi)$, *and suppose that* V *satisfies* (4.1). *Let* H_{θ_0,θ_R} *and* $H_{\theta_0',\theta_R'}$ *be defined as in* (3.5). *Then,*

$$\begin{aligned}
&\operatorname{tr}_{L^2((0,R);dx)}\big((H_{\theta_0',\theta_R'} - zI)^{-1} - (H_{\theta_0,\theta_R} - zI)^{-1}\big) \\
&\quad = -\operatorname{tr}_{\mathbb{C}^2}\left(\left[\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\right]^{-1} \frac{d}{dz}\left[\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\right]\right) \\
&\quad = -\frac{d}{dz}\ln\Big(\operatorname{det}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)\Big), \quad z \in \mathbb{C}\backslash[e_0, \infty).
\end{aligned} \tag{5.3}$$

If, in addition, $\theta_0', \theta_R' \in (0, 2\pi)\backslash\{\pi\}$, *then*

$$\begin{aligned}
&\operatorname{tr}_{L^2((0,R);dx)}\big((H_{\theta_0',\theta_R'} - zI)^{-1} - (H_{\theta_0,\theta_R} - zI)^{-1}\big) \\
&= -\frac{d}{dz}\ln\Big(\operatorname{det}_{L^2((0,R);dx)}\Big(\overline{(H_{\theta_0',\theta_R'} - zI)^{1/2}(H_{\theta_0,\theta_R} - zI)^{-1}(H_{\theta_0',\theta_R'} - zI)^{1/2}}\Big)\Big), \\
&\qquad\qquad z \in \mathbb{C}\backslash[e_0, \infty).
\end{aligned} \tag{5.4}$$

Proof. The second equality in (5.3) is obvious. Next, we temporarily suppose that $\theta_0 \neq \theta_0'$ and $\theta_R \neq \theta_R'$. Then the first equality in (5.3) follows upon taking the trace in (3.76), using cyclicity of the trace, and applying (5.1) (keeping in mind that $S_{\theta_0'-\theta_0,\theta_R'-\theta_R}$ is invertible and z-independent). The remaining cases where $\theta_0 = \theta_0'$ or $\theta_R = \theta_R'$ follow similarly (the case where $\theta_0 = \theta_0'$ and $\theta_R = \theta_R'$ instantly follows from (3.25)).

Relation (5.4) follows from (2.57), (4.16), and (5.3). □

Next, we note that the rank-two behavior of the difference of the resolvents of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ displayed in Theorem 3.11 permits one to define the spectral shift function $\xi(\,\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$ associated with the pair $(H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$. Using the standard normalization in the context of self-adjoint operators bounded from below,

$$\xi(\,\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R}) = 0, \quad \lambda < e_0 = \inf\big(\sigma(H_{\theta_0,\theta_R}) \cup \sigma(H_{\theta_0',\theta_R'})\big), \tag{5.5}$$

Krein's trace formula (see, e.g., [72, Ch. 8], [73]) reads

$$\begin{aligned}
&\operatorname{tr}_{L^2((0,R);dx)}\big((H_{\theta_0',\theta_R'} - zI)^{-1} - (H_{\theta_0,\theta_R} - zI)^{-1}\big) \\
&\quad = -\int_{[e_0,\infty)} \frac{\xi(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})\, d\lambda}{(\lambda - z)^2}, \quad z \in \rho(H_{\theta_0,\theta_R}) \cap \rho(H_{\theta_0',\theta_R'})\big),
\end{aligned} \tag{5.6}$$

where $\xi(\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$ satisfies

$$\xi(\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R}) \in L^1\big(\mathbb{R}; (\lambda^2 + 1)^{-1} d\lambda\big). \tag{5.7}$$

Since the spectra of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ are purely discrete, $\xi(\,\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$ is a piecewise constant function on $\mathbb{R}$ with jumps at the eigenvalues of H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$, the jumps corresponding to the multiplicity of the eigenvalue in question.

Moreover, $\xi(\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$ permits a representation in terms of nontangential boundary values to the real axis of $\operatorname{det}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\cdot)\Big)$ (resp., of the symmetrized perturbation determinant (4.14)), to be described in Theorem 5.3.

Since by (3.8) and (3.9) it suffices to consider $\theta_0, \theta_R \in [0, \pi)$ when considering the operator H_{θ_0,θ_R}, we will restrict the boundary condition parameters accordingly next:

Theorem 5.3. *Assume that $\theta_0, \theta_R \in [0,\pi)$, $\theta_0', \theta_R' \in (0,\pi)$, and suppose that V satisfies* (4.1). *Let H_{θ_0,θ_R} and $H_{\theta_0',\theta_R'}$ be defined as in* (3.5). *Then,*

$$\xi(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R}) = \pi^{-1} \lim_{\varepsilon\downarrow 0} \operatorname{Im}\Big(\ln\Big(\eta(\theta_0,\theta_R) \det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(\lambda+i\varepsilon)\Big)\Big)\Big) \quad \text{for a.e. } \lambda\in\mathbb{R}, \tag{5.8}$$

where

$$\eta(\theta_0,\theta_R) = \begin{cases} 1, & \theta_0,\theta_R \in (0,\pi),\ \theta_0=\theta_R=0, \\ -1, & \theta_0=0,\ \theta_R\in(0,\pi),\ \theta_0\in(0,\pi),\ \theta_R=0. \end{cases} \tag{5.9}$$

Proof. We recall the definition of $e_0 = \inf\big(\sigma(H_{\theta_0,\theta_R}) \cup \sigma(H_{\theta_0',\theta_R'})\big)$ in (5.5).

Combining (5.3) and (5.6) one obtains

$$\frac{d}{dz}\ln\Big(\eta(\theta_0,\theta_R) \det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)\Big) = \int_{[e_0,\infty)} \frac{\xi(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})\, d\lambda}{(\lambda-z)^2}, \quad z\in\rho(H_{\theta_0,\theta_R})\cap\rho(H_{\theta_0',\theta_R'}), \tag{5.10}$$

since $\eta(\theta_0,\theta_R)$ is z-independent.

Next, combining (3.39) and (3.49), and using the fact that $\phi(z,x)$ and $\theta(z,x)$ are both real-valued for $z,x\in\mathbb{R}$, one concludes that $\Delta(z,R,\theta_0,\theta_R)$, and hence $\det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)$ are real-valued for $z\in\mathbb{R}$ and $\theta_0,\theta_R,\theta_0',\theta_R'\in[0,\pi)$. Moreover, using the fact that

$$\det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big) \neq 0, \quad z<e_0, \tag{5.11}$$

and invoking the asymptotic behavior (3.53) as $z\downarrow 0$, one actually concludes that

$$\det_{\mathbb{C}^2}\Big(\eta(\theta_0,\theta_R)\,\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big) > 0, \quad z<e_0. \tag{5.12}$$

Integrating (5.10) with respect to the z-variable along the real axis from z_0 to z, assuming $z<z_0<e_0$, one obtains

$$\begin{aligned}
&\ln\Big(\eta(\theta_0,\theta_R) \det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)\Big) - \ln\Big(\eta(\theta_0,\theta_R) \det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z_0)\Big)\Big) \\
&\quad = \int_{z_0}^{z} d\zeta \int_{[e_0,\infty)} \frac{\xi(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})\, d\lambda}{(\lambda-\zeta)^2} \\
&\quad = \int_{z_0}^{z} d\zeta \int_{[e_0,\infty)} \frac{[\xi_+(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R}) - \xi_-(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})]\, d\lambda}{(\lambda-\zeta)^2} \\
&\quad = \int_{[e_0,\infty)} [\xi_+(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R}) - \xi_-(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})]\, d\lambda \int_{z_0}^{z} \frac{d\zeta}{(\lambda-\zeta)^2} \\
&\quad = \int_{[e_0,\infty)} \xi(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})\, d\lambda \bigg(\frac{1}{\lambda-z} - \frac{1}{\lambda-z_0}\bigg), \quad z<z_0<e_0.
\end{aligned} \tag{5.13}$$

Here we split ξ into its positive and negative parts, $\xi_\pm = [|\xi|\pm\xi]/2$, and applied the Fubini–Tonelli theorem to interchange the integrations with respect to λ and ζ. Moreover, we chose the branch of $\ln(\cdot)$ such that $\ln(x)\in\mathbb{R}$ for $x>0$, compatible with the normalization of $\xi(\,\cdot\,; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})$ in (5.5).

An analytic continuation of the first and last line of (5.13) with respect to z then yields

$$\ln\Big(\eta(\theta_0,\theta_R) \det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z)\Big)\Big) - \ln\Big(\eta(\theta_0,\theta_R) \det_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z_0)\Big)\Big)$$

$$= \int_{[e_0,\infty)} \xi(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})\, d\lambda \bigg(\frac{1}{\lambda - z} - \frac{1}{\lambda - z_0}\bigg), \quad z \in \mathbb{C}\backslash[e_0,\infty). \quad (5.14)$$

Since by (5.12),

$$\ln\Big(\eta(\theta_0,\theta_R)\det{}_{\mathbb{C}^2}\Big(\Lambda_{\theta_0,\theta_R}^{\theta_0',\theta_R'}(z_0)\Big)\Big) \in \mathbb{R}, \quad z_0 < e_0, \quad (5.15)$$

the Stieltjes inversion formula separately applied to the absolutely continuous measures $\xi_\pm(\lambda; H_{\theta_0',\theta_R'}, H_{\theta_0,\theta_R})\, d\lambda$ (cf., e.g., [5, p. 328], [71, App. B]), then yields (5.8). □

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